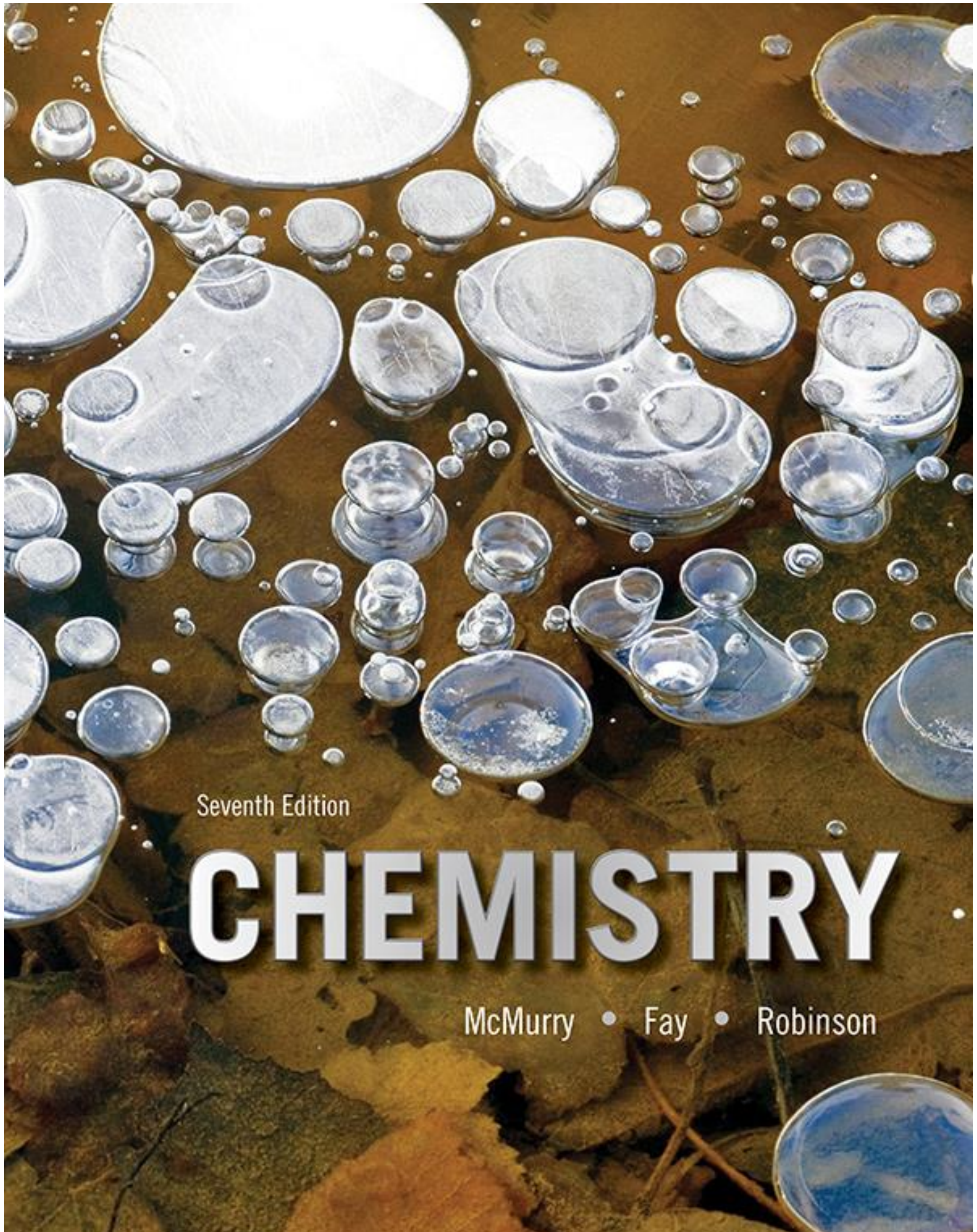


Lecture Presentation

Chapter 8
Covalent Compounds: Bonding Theories and Molecular Structure

8.1, 8.2, 8.3, 8.4, 8.5, 8.6, 8.7, 8.8, 8.9, 8.10, 8.11, 8.12, 8.13, 8.16, 8.17, 8.18, 8.19, 8.20, 8.21, 8.22, 8.23, 8.24, 8.6, 8.28, 8.34, 8.42, 8.44, 8.46, 8.48, 8.52, 8.54, 8.60, 8.62, 8.66, 8.72, 8.74, 8.76, 8.86, 8.88, 8.94, 8.100

John E. McMurry
Robert C. Fay

Molecular Shapes: The VSEPR Model

Valence Shell Electron Pair Repulsion [VSEPRT (theory)]

Step 1

- Draw an electron-dot structure (Lewis Dot Structure) for the molecule, & count the number of **electron charge clouds (my handout calls these e domain or e pairs)** surrounding the atom of interest.

Step 2

- Predict the geometric arrangement of charge clouds by assuming that the charge clouds are oriented in space as far away from each other as possible. (like tying together balloons) – Can see atoms. Can't see lone pair e.

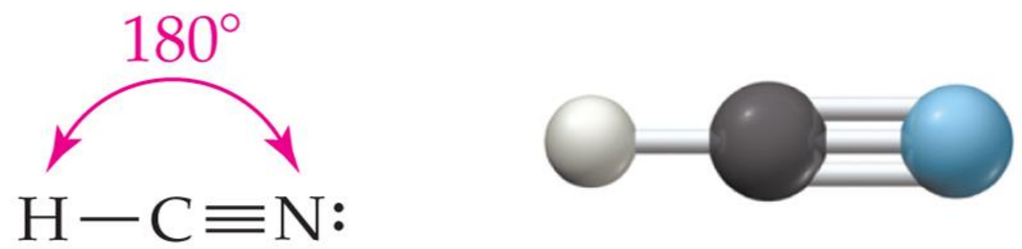
- A+ point: lone pairs (nonbonding e) occupy slightly more space than bonding e (slightly larger bond angle around nonbonding e)

Molecular Shapes: The VSEPR Model

Two Charge Clouds

A CO_2 molecule is linear, with a bond angle of 180°.

An HCN molecule is linear, with a bond angle of 180°.

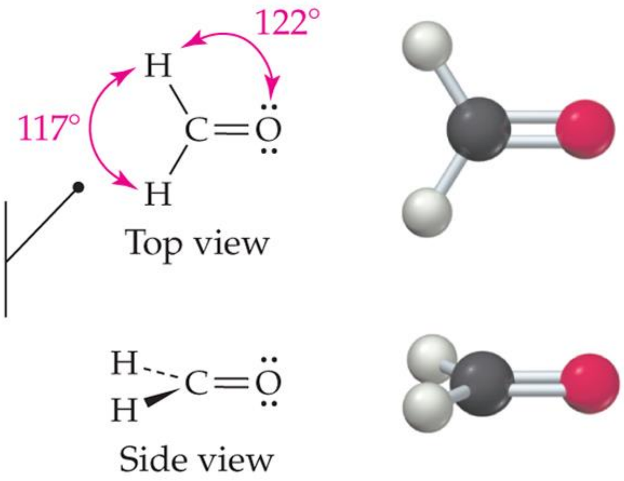


Note: single, double and triple bonds counts as ONE charge cloud (like balloons tied down on two sides by atoms)

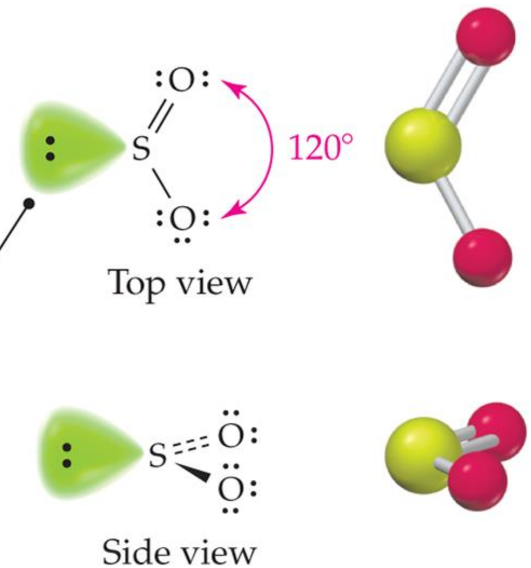
Molecular Shapes: The VSEPR Model

Three Charge Clouds

A formaldehyde molecule is trigonal planar, with bond angles of roughly 120°.

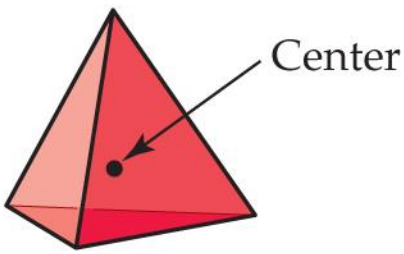


An SO_2 molecule is bent, with a bond angle of approximately 120°.



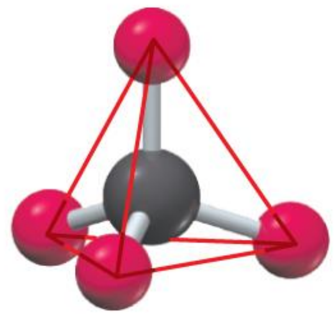
Molecular Shapes: The VSEPR Model

Four Charge Clouds

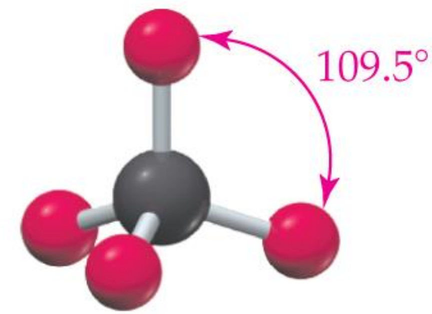


A regular tetrahedron

The atom is located in the **center** of a regular tetrahedron.



The four charge clouds point to the **four corners** of the tetrahedron.



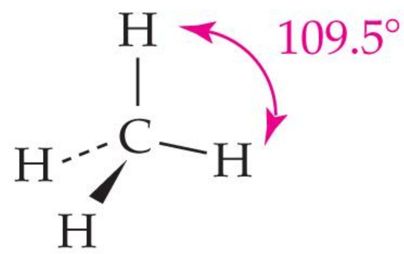
A tetrahedral molecule

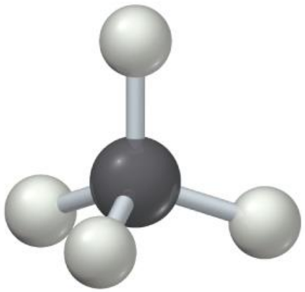
The angle between any two bonds is 109.5°.

Molecular Shapes: The VSEPR Model

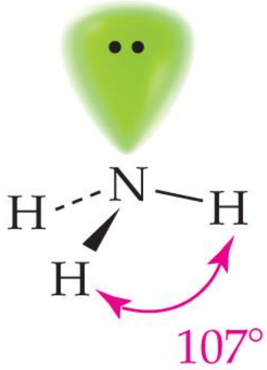
Four Charge Clouds

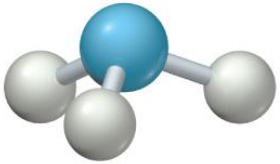
A methane molecule is tetrahedral, with bond angles of 109.5°.



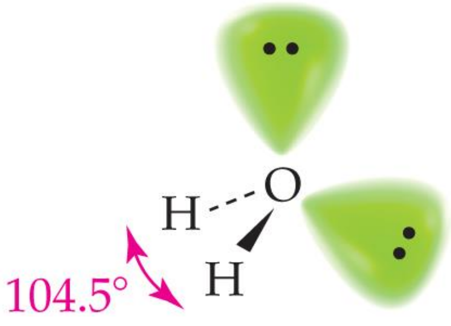


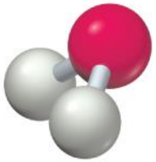
An ammonia molecule is trigonal pyramidal, with bond angles of 107°.





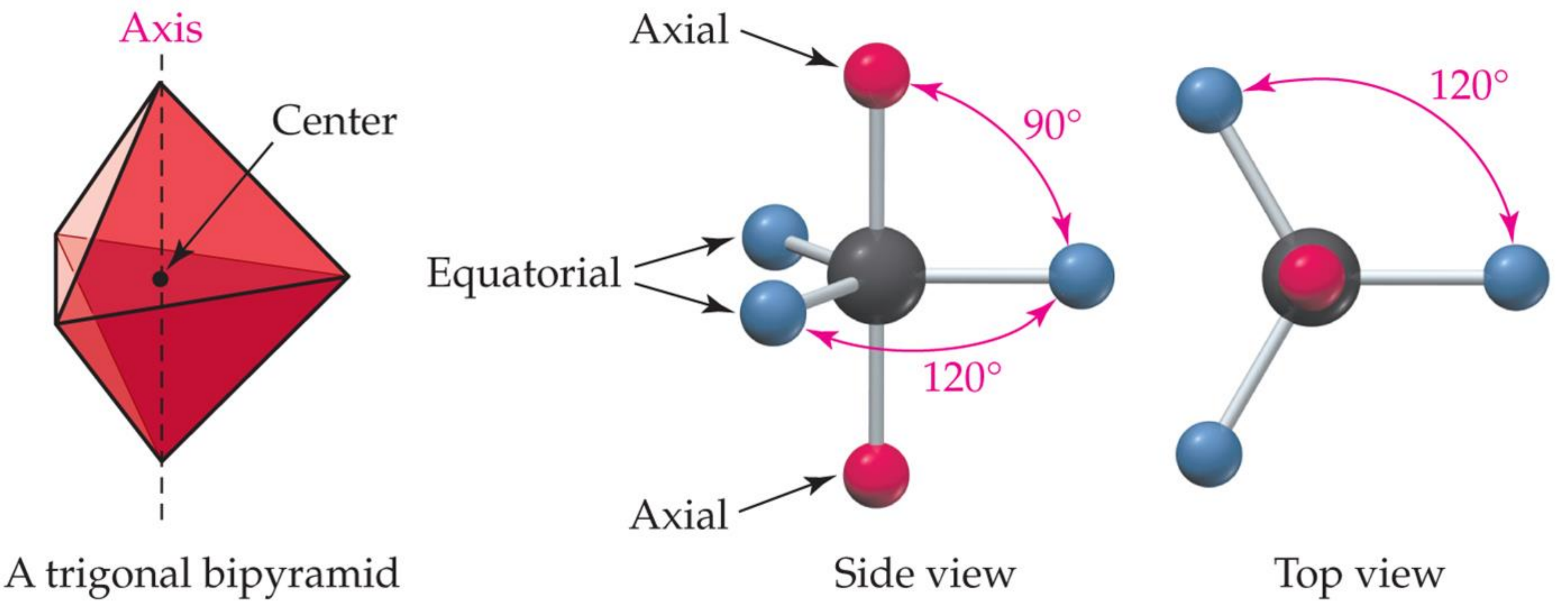
A water molecule is bent, with a bond angle of 104.5°.





Molecular Shapes: The VSEPR Model

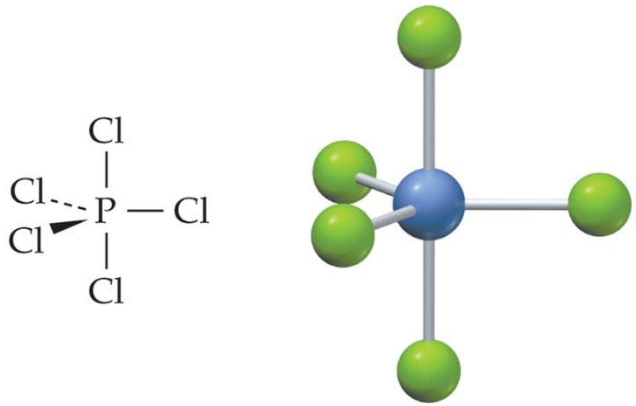
Five Charge Clouds

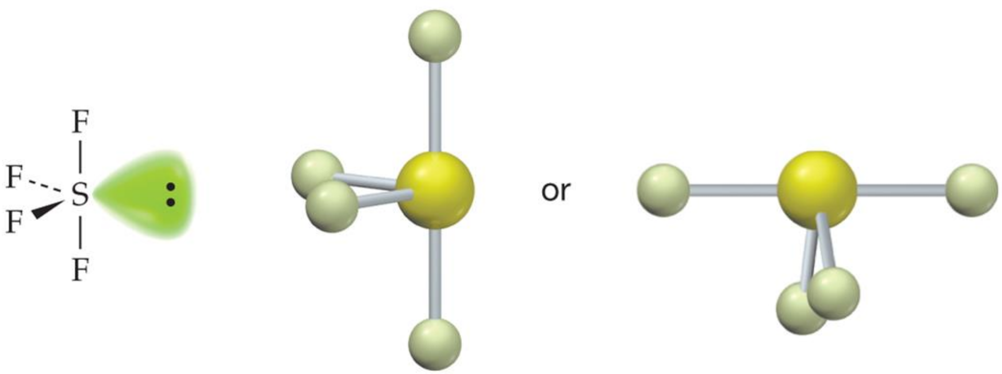


Molecular Shapes: The VSEPR Model

Five Charge Clouds

A PCl_5 molecule is trigonal bipyramidal.



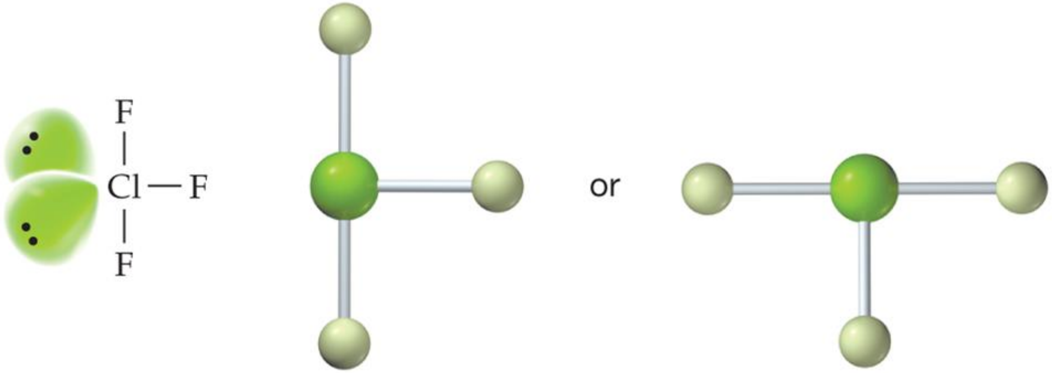


In this orientation, an SF_4 molecule takes on a shape like a seesaw.

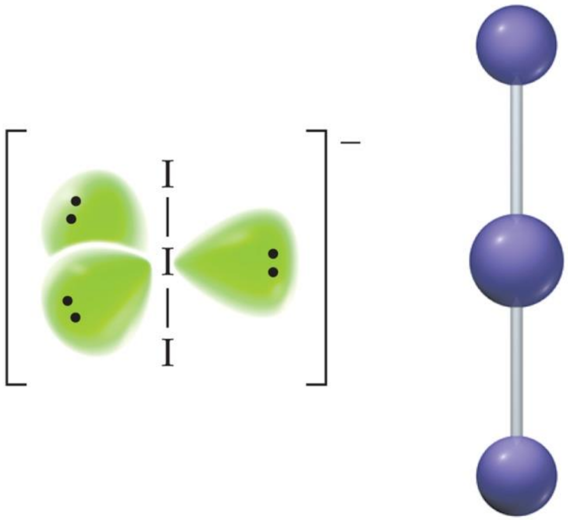
Molecular Shapes: The VSEPR Model

Five Charge Clouds

A ClF_3 molecule is T-shaped.

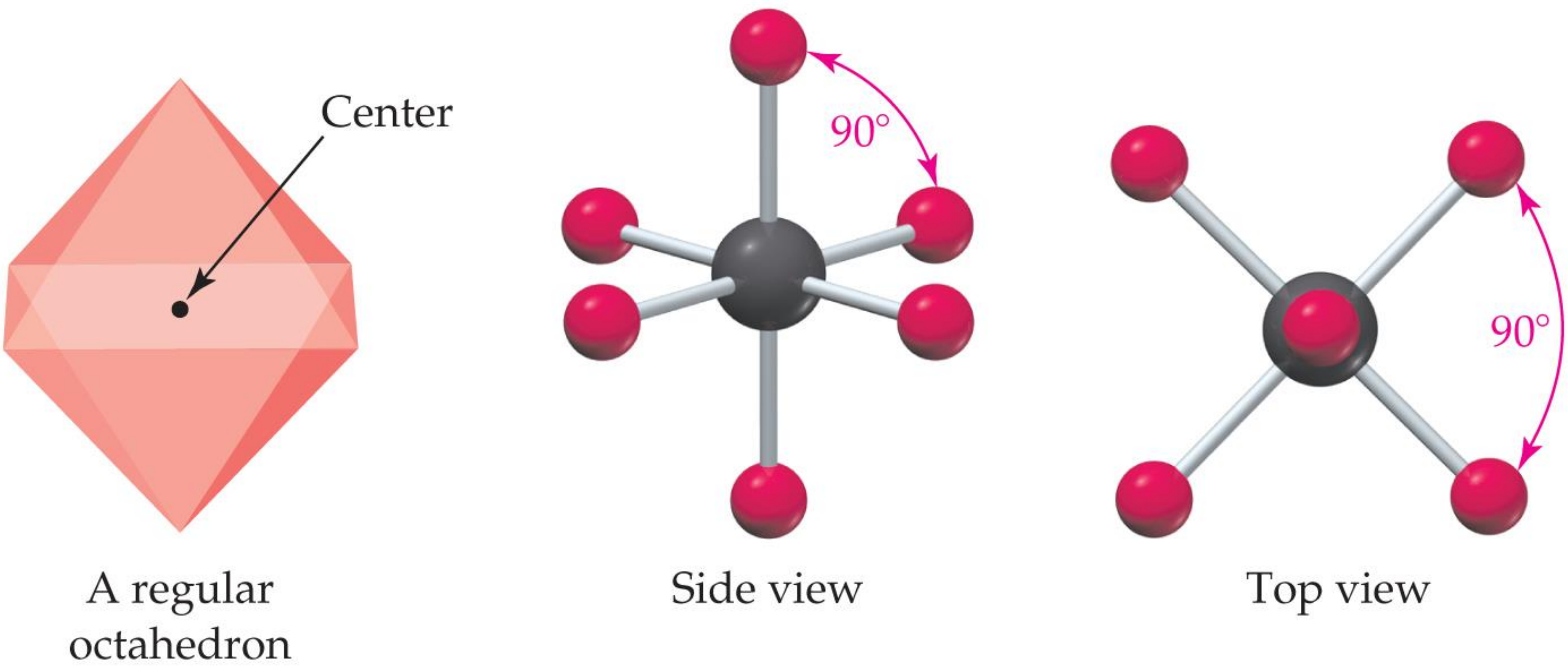


An I_3^- ion is linear.



Molecular Shapes: The VSEPR Model

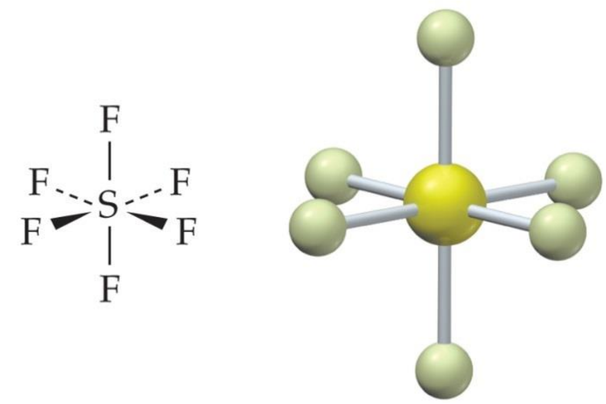
Six Charge Clouds



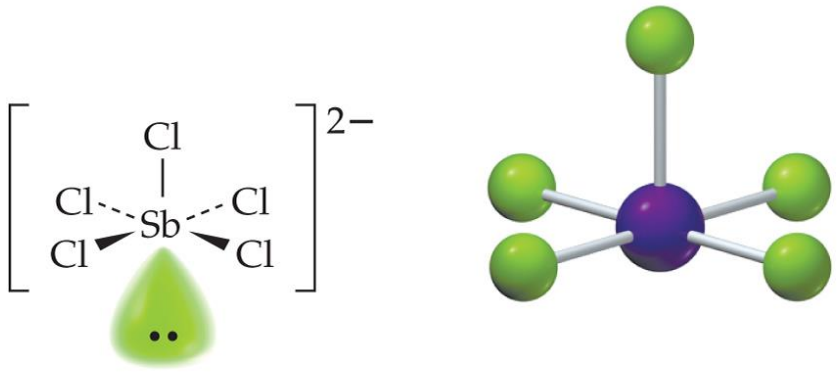
Molecular Shapes: The VSEPR Model

Six Charge Clouds

An SF_6 molecule is octahedral.



An $SbCl_5^{2-}$ ion has a square pyramidal shape.



Molecular Shapes: The VSEPR Model

Six Charge Clouds

An XeF_4 molecule has a square planar shape.

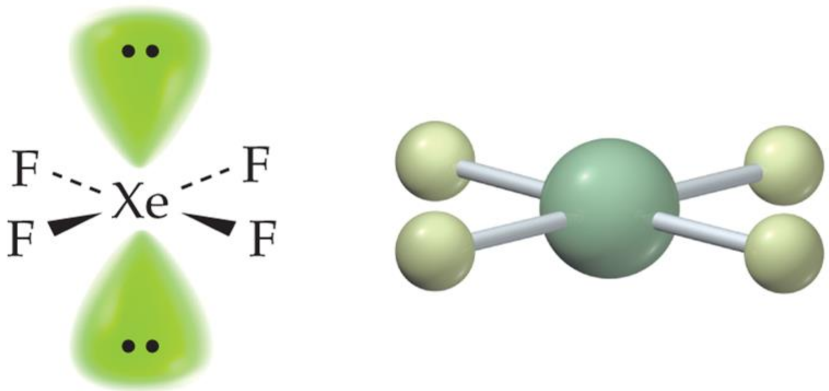
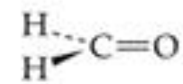
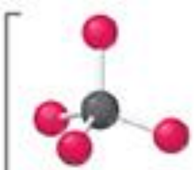
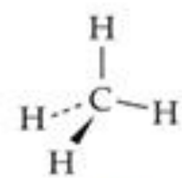
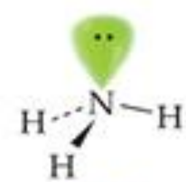
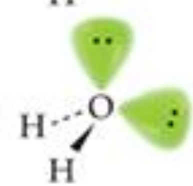
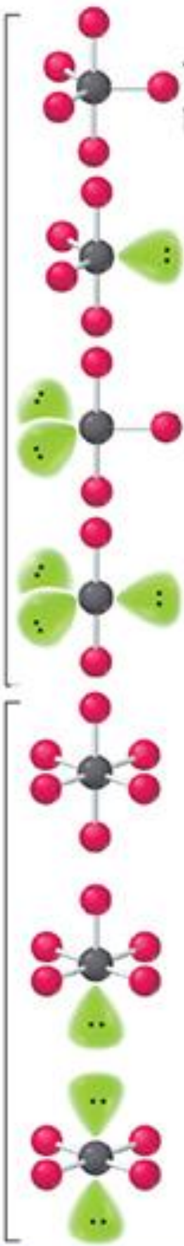
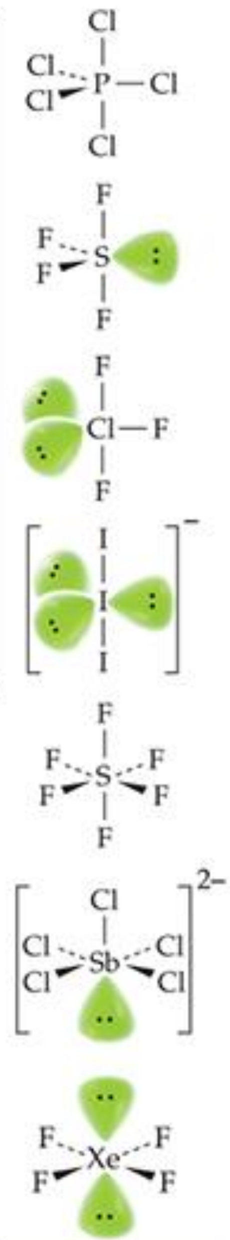


TABLE 8.1 Geometry Around Atoms with 2, 3, 4, 5, and 6 Charge Clouds

Number of Bonds	Number of Lone Pairs	Number of Charge Clouds	Geometry and Shape	Example
2	0	2	 Linear	O=C=O
3	0	3	 Trigonal planar	
2	1		 Bent	
4	0		 Tetrahedral	
3	1	4	 Trigonal pyramidal	
2	2		 Bent	

5	0	5	Trigonal bipyramidal
4	1	5	Seesaw
3	2	5	T-shaped
2	3	5	Linear
6	0	6	Octahedral
5	1	6	Square pyramidal
4	2	6	Square planar





To do VSEPRT (using chart next slide & handout)

1. Draw Electron Dot Structure (Lewis Dot Structure).

2. # charge clouds (# e pairs/e domains) = # bonds + # lone pairs

 # of bonds to central atom (single, double and triple bonds count as one bond for VSEPRT)

(# of lone pairs on the central atom - not # of electrons in lone pairs but # of pairs)

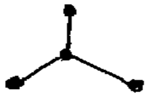
3. Use geometry e pairs & geometry of molecule for VSEPRT (# lone pairs/nonbonding e – these e are invisible for molecular shape)

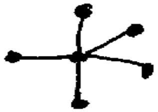
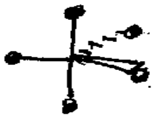
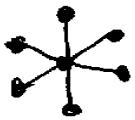
11/15 F section Friday

4. Use hybridization for Valence Bond

VSEPR & valence bond hybrization chart (e pair/domains = charge cloud)

# electron pairs(domains)	# lone pair	hybridization	geometry of electron pairs	geometry of molecules	angles
2	0	sp	linear	linear	180
3	0	sp^2	trigonal planar	trigonal planar	120
3	1	sp^2	trigonal planar	bent	
3	2	sp^2	trigonal planar	linear	
4	0	sp^3	tetrahedral	tetrahedral	109.5
4	1	sp^3	tetrahedral	trigonal pyramidal	
4	2	sp^3	tetrahedral	bent	
4	3	sp^3	tetrahedral	linear	
5	0	sp^3d	trigonal bipyramidal	trigonal bipyramidal	120 & 90
5	1	sp^3d	trigonal bipyramidal	see saw	
5	2	sp^3d	trigonal bipyramidal	T shaped	
5	3	sp^3d	trigonal bipyramidal	linear	
6	0	sp^3d^2	octahedral	octahedral	90
6	1	sp^3d^2	octahedral	square pyramidal	
6	2	sp^3d^2	octahedral	square planar	
6	3	sp^3d^2	octahedral	T shaped	
6	4	sp^3d^2	octahedral	bent	




HW 8-1: Do VSEPRT (on central atom)

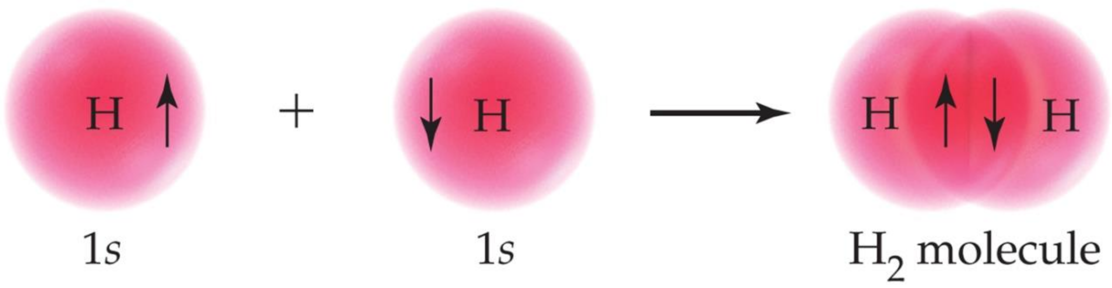
Note: I now do NOT post the HW or HW answers with the posted powerpoint. You can come to class and pick up the HW powerpoint handout for in this case HW 8-1. You will have to get the answers to HW from either a fellow student who was in class OR get the answer from me by asking questions. I usually give the answer at the next class period as well.

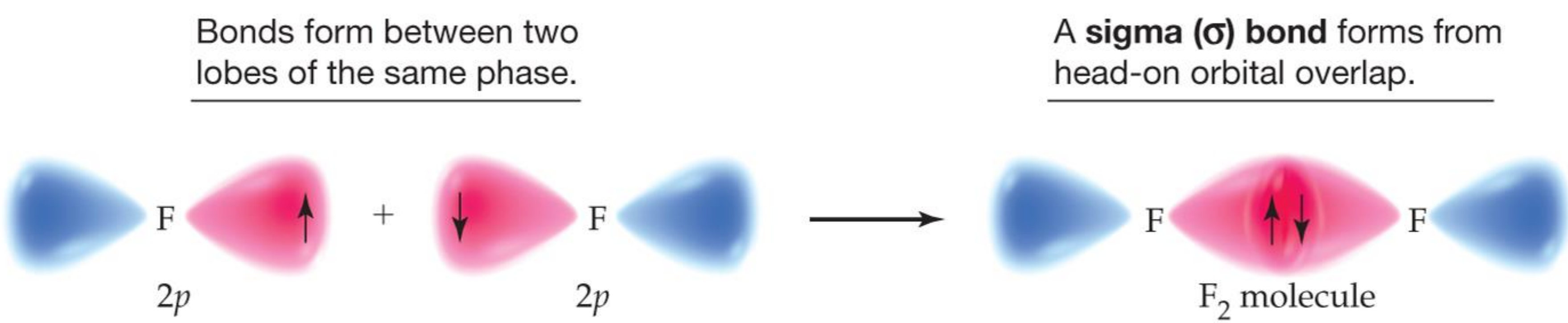
11/15 Friday G section

11/18 Monday D section

Valence Bond Theory

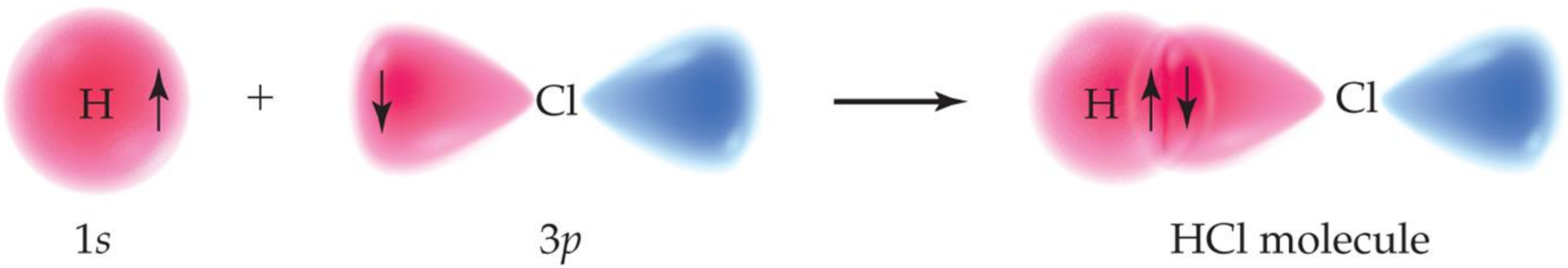
Valence Bond Theory: A quantum mechanical model that shows how electron pairs are shared in a covalent bond





Valence Bond Theory

Valence Bond Theory: A quantum mechanical model that shows how electron pairs are shared in a covalent bond



Valence Bond Theory

- Covalent bonds are formed by overlap of atomic orbitals, each of which contains one electron of opposite spin.

- Each of the bonded atoms keep its own atomic orbitals, but the electron pair in the overlapping orbitals is shared by both atoms.

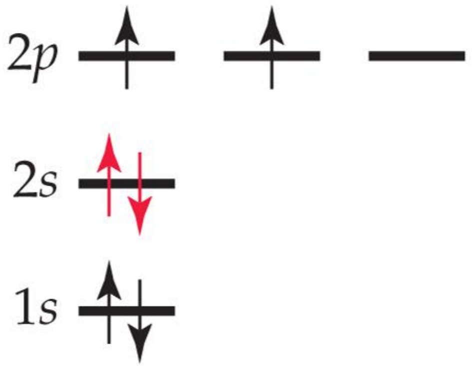
- The greater the amount of overlap, the stronger the bond.

Hybridization and *sp*^{3} Hybrid Orbitals

How can the bonding in CH_4 be explained?

4 valence electrons

2 unpaired electrons

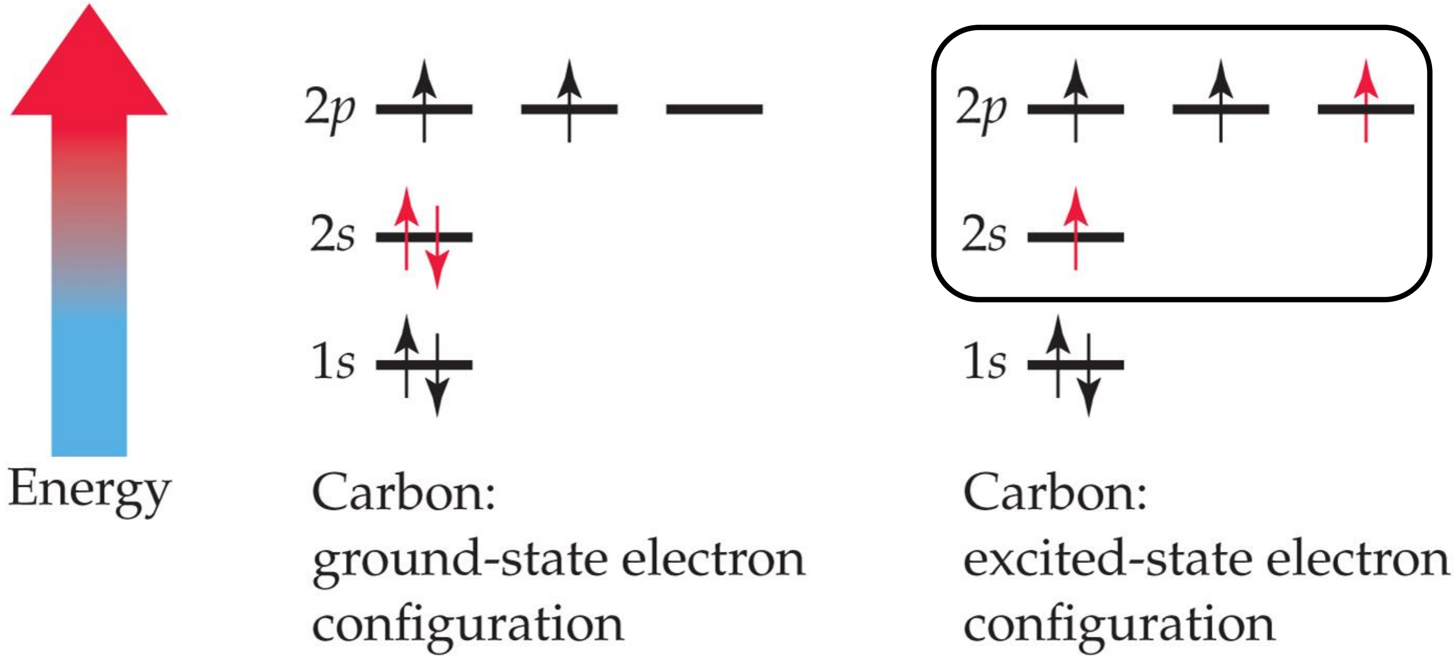


Carbon:
ground-state electron configuration

Hybridization and sp^3 Hybrid Orbitals

How can the bonding in CH_4 be explained?

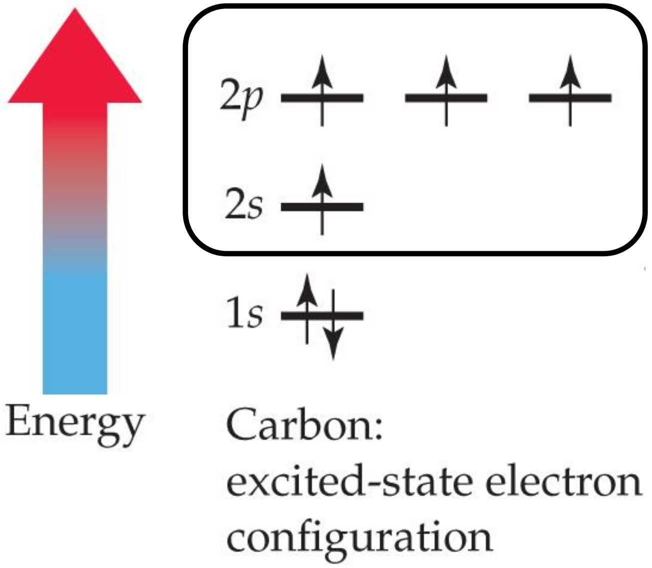
4 valence electrons
2 unpaired electrons



Hybridization and sp^3 Hybrid Orbitals

How can the bonding in CH_4 be explained?

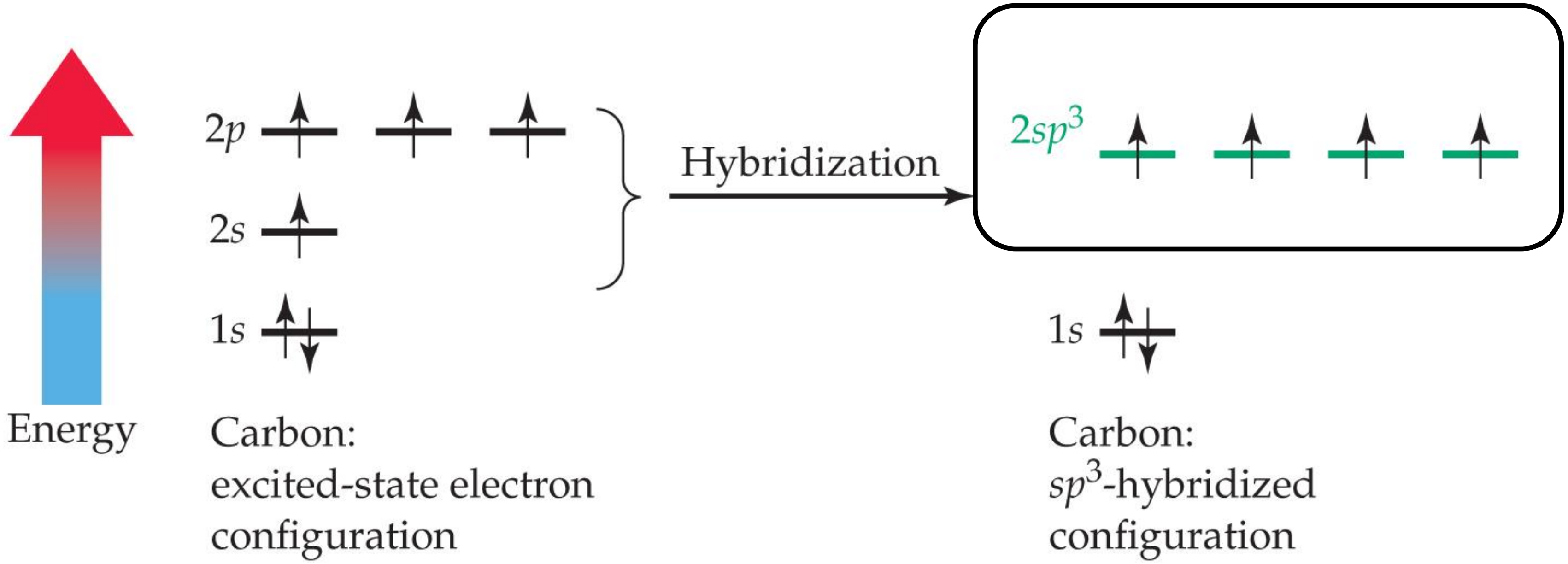
4 **nonequivalent** orbitals



Hybridization and *sp*^{3} Hybrid Orbitals

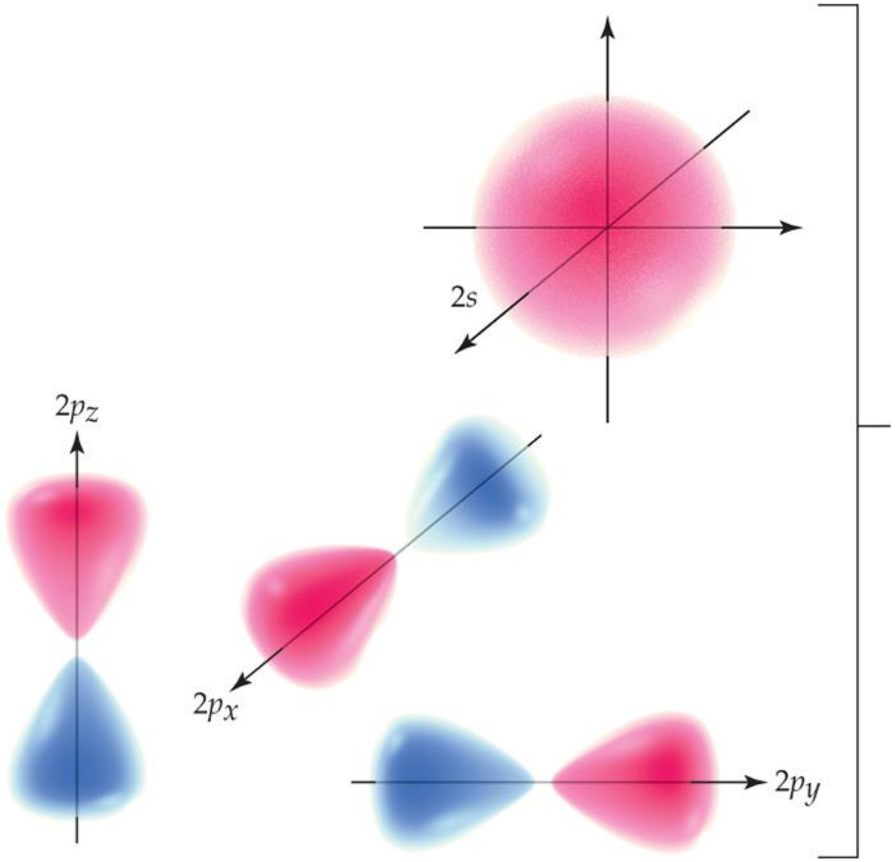
How can the bonding in CH_4 be explained?

4 **equivalent** orbitals



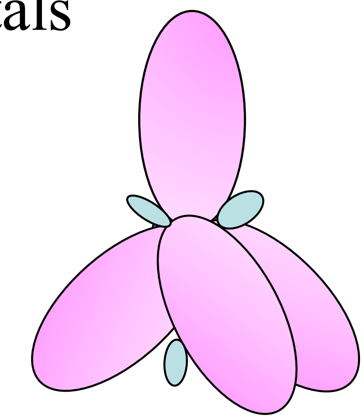
1s + 3 p = 4 sp3 orbitals

Other Kinds of Hybrid Orbitals – sp^3 orbitals



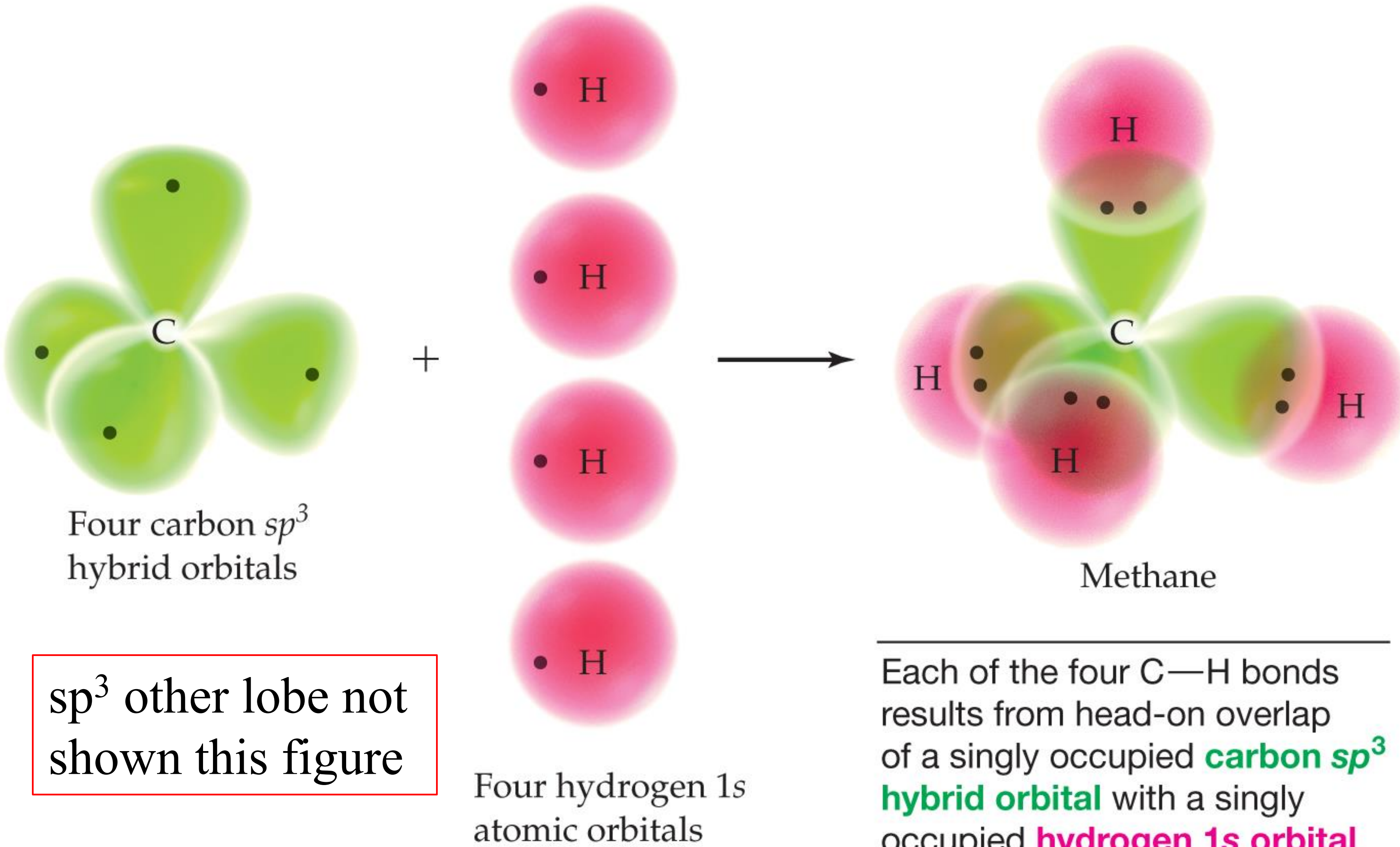
sp^3

4 sp^3 orbitals



Your text's powerpoint figure is incorrect (gave sp^2 fig). My version is shown above. sp^3 looks like p but with one lobe smaller than other.

Hybridization 4 sp^3 Hybrid Orbitals + 4 s orbitals

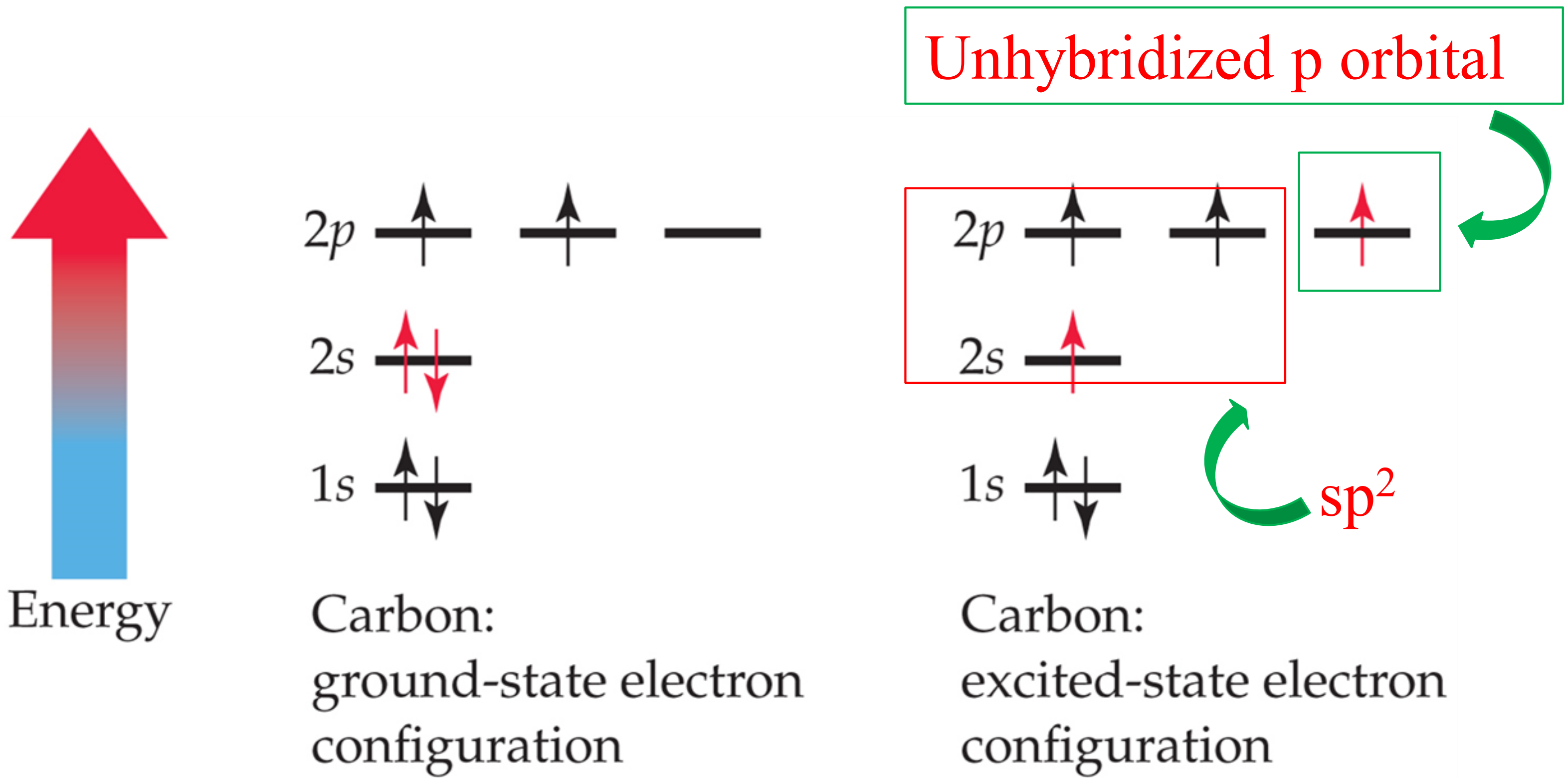


Each of the four C—H bonds results from head-on overlap of a singly occupied **carbon sp^3 hybrid orbital** with a singly occupied **hydrogen 1s orbital**.

sp^3 other lobe not shown this figure

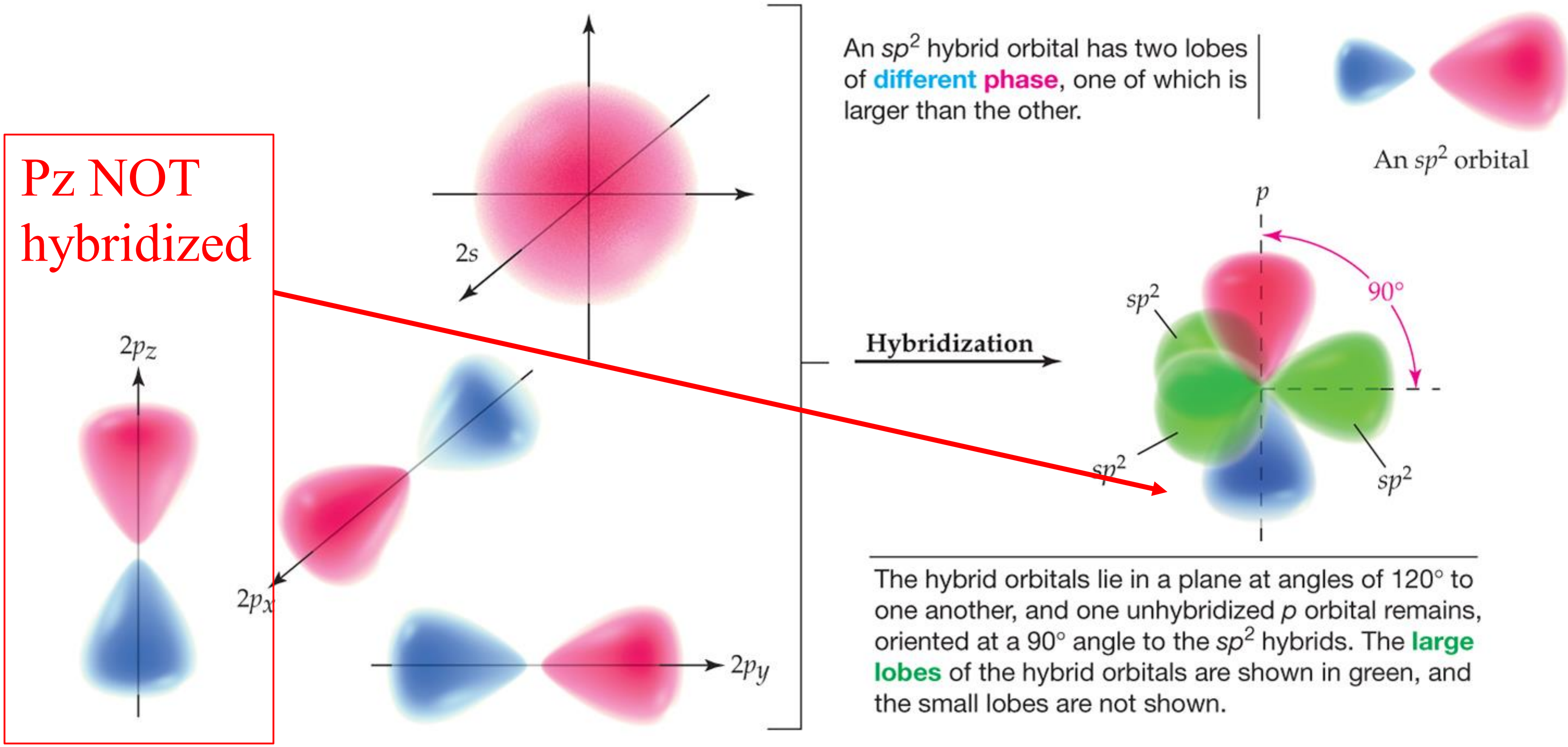
Hybridization and sp^2 Hybrid Orbitals

How can the bonding in $CH_2 = CH_2$ be explained?
(starts out same as orbital diagram for sp^3)

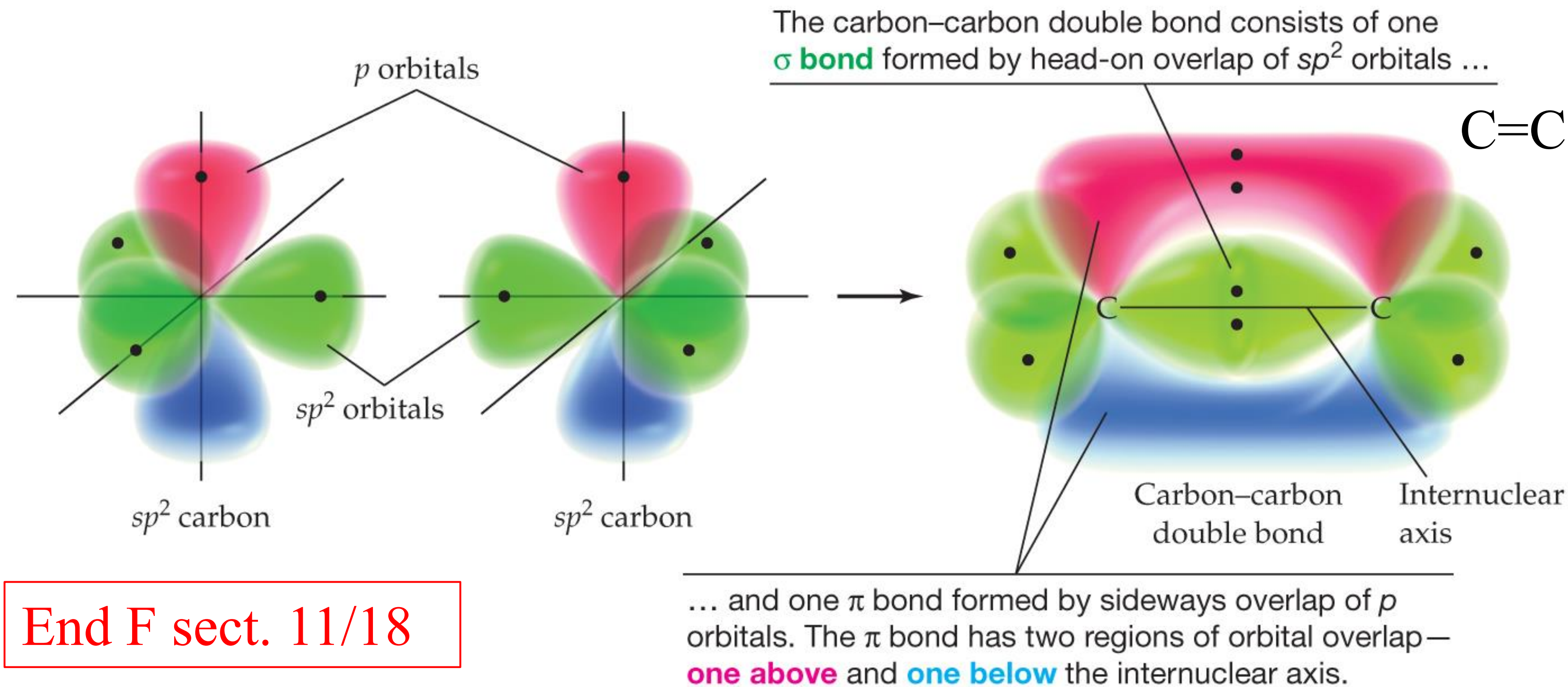


1s + 2p = 3 sp2 + 1 unhybridized p

Other Kinds of Hybrid Orbitals – sp^2



Other Kinds of Hybrid Orbitals – sp^2



End F sect. 11/18

σ bond overlaps head on in plane

π bond overlaps sideways with no electron density in between atoms (like a doughnut)

HW: 8-2

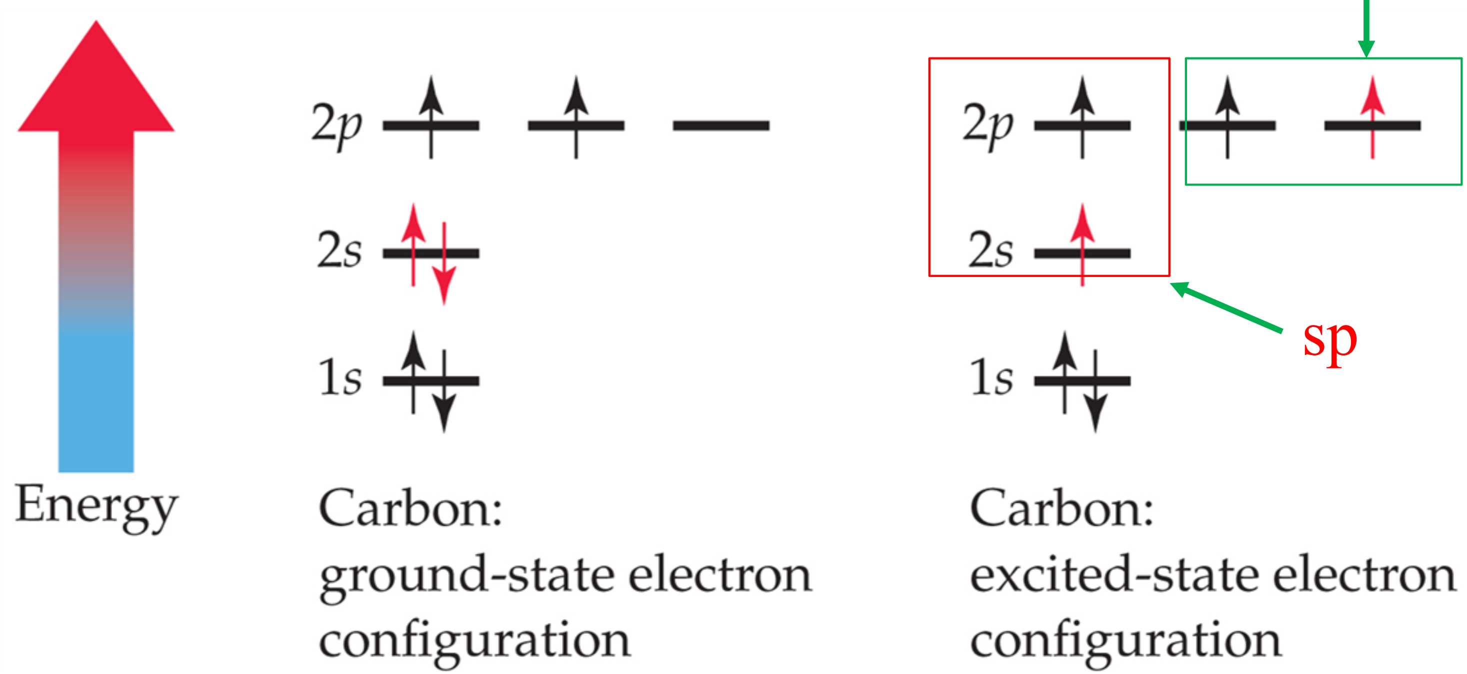
Note: I now do NOT post the HW or HW answers with the posted powerpoint. You can come to class and pick up the HW powerpoint handout for in this case HW 8-2. You will have to get the answers to HW from either a fellow student who was in class OR get the answer from me by asking questions. I usually give the answer at the next class period as well.

Hybridization and *sp* Hybrid Orbitals

How can the bonding in $CH \equiv CH$ be explained?

End 11/18 Monday
G sect

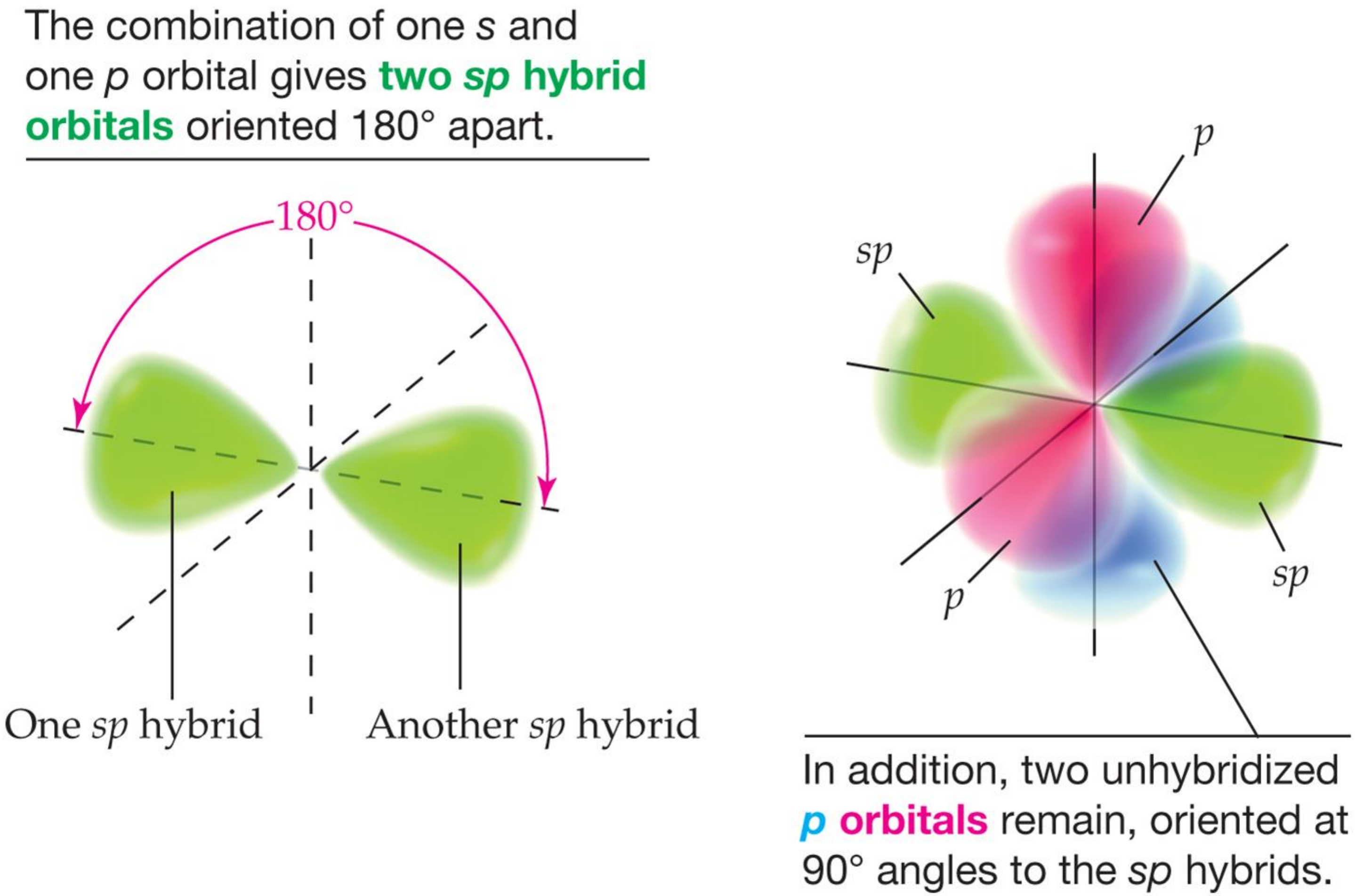
Unhybridized p orbitals



1s+1p = 2 sp + 2 unhybridized p

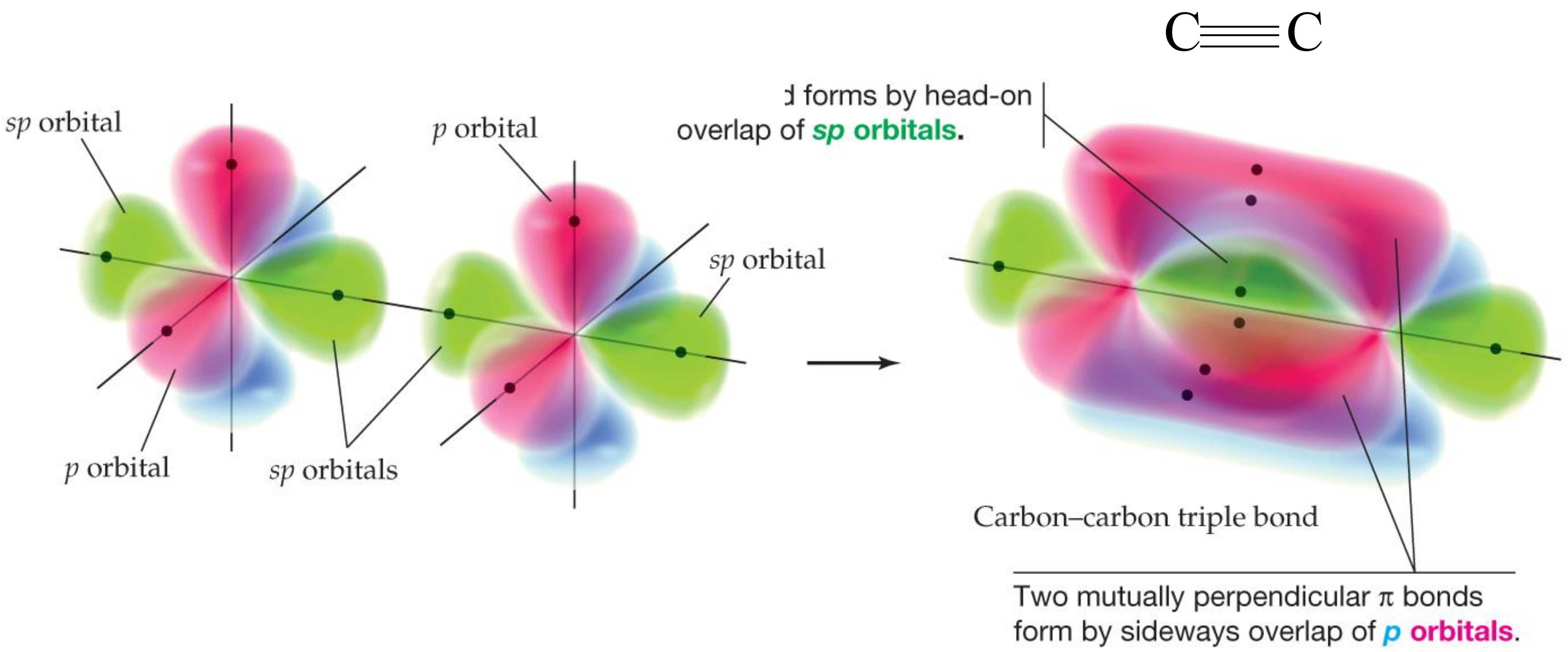
Other Kinds of Hybrid Orbitals –

2 hybridized sp orbitals + 2 unhybridized p



Other Kinds of Hybrid Orbitals –

2 hybridized sp orbitals + 2 unhybridized p



11/20 Wednesday D section

HW: 8-3

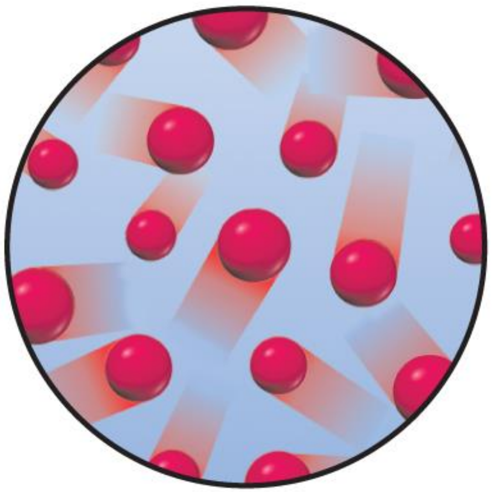
Note: I now do NOT post the HW or HW answers with the posted powerpoint. You can come to class and pick up the HW powerpoint handout for in this case HW 8-3. You will have to get the answers to HW from either a fellow student who was in class OR get the answer from me by asking questions. I usually give the answer at the next class period as well.

Other Kinds of Hybrid Orbitals

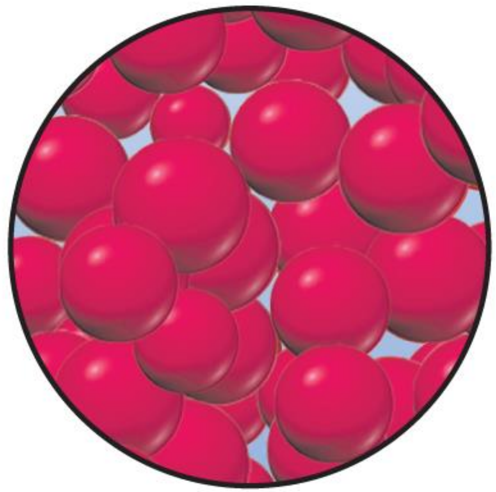
TABLE 8.2 Hybrid Orbitals and Their Geometry

Number of Charge Clouds	Arrangement of Charge Clouds	Hybridization
2	Linear	*sp*
3	Trigonal planar	sp^2
4	Tetrahedral	sp^3

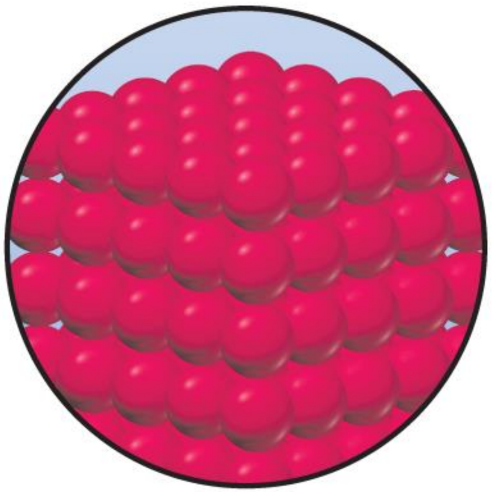
Polar Covalent Bonds and Dipole Moments



In **gases**, the particles feel little attraction for one another and are free to move about randomly.

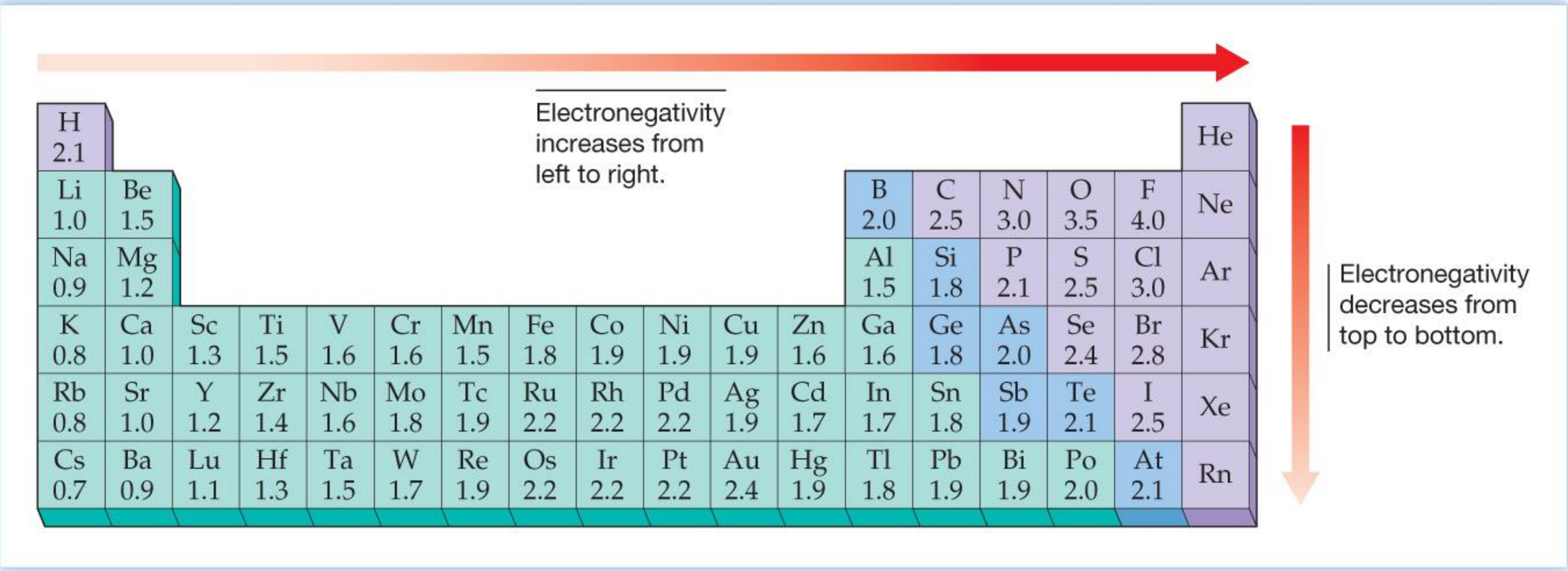


In **liquids**, the particles are held close together by attractive forces but are free to move around one another.

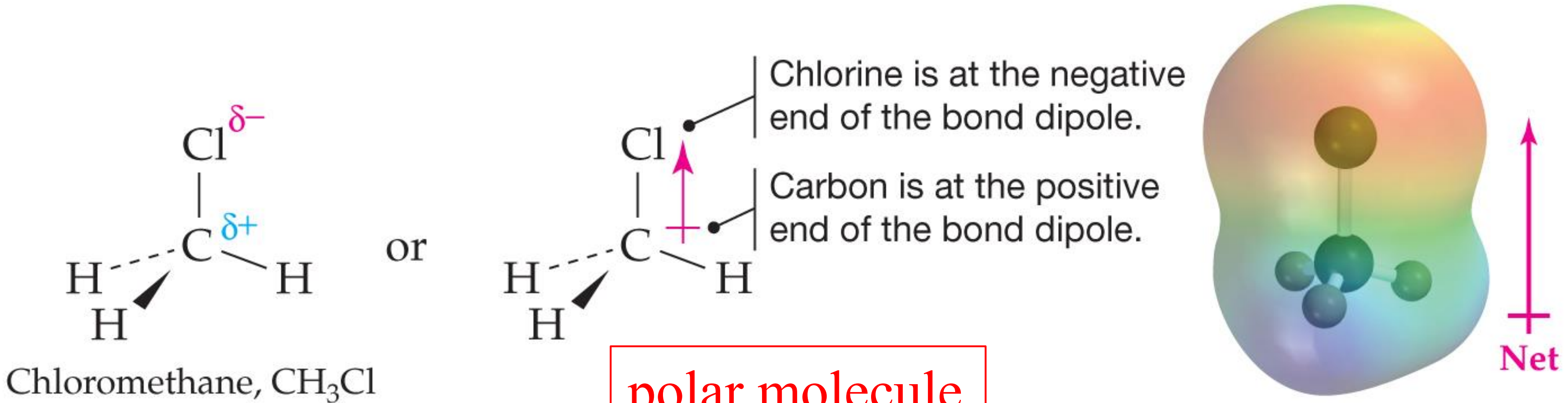


In **solids**, the particles are held in an ordered arrangement.

Polar Covalent Bonds and Dipole Moments



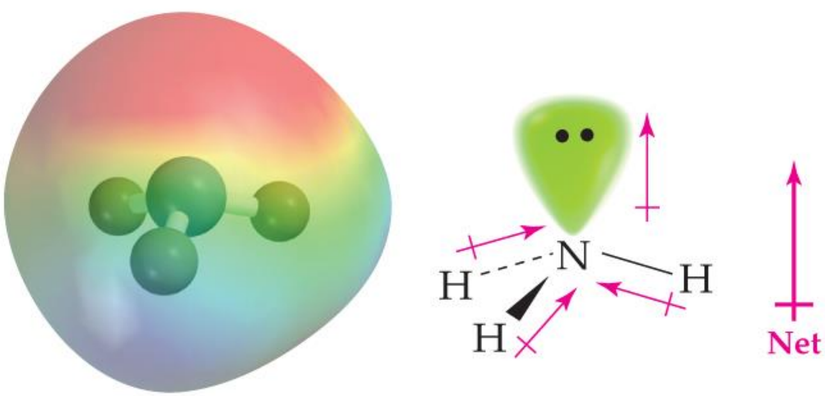
Polar Covalent Bonds and Dipole Moments



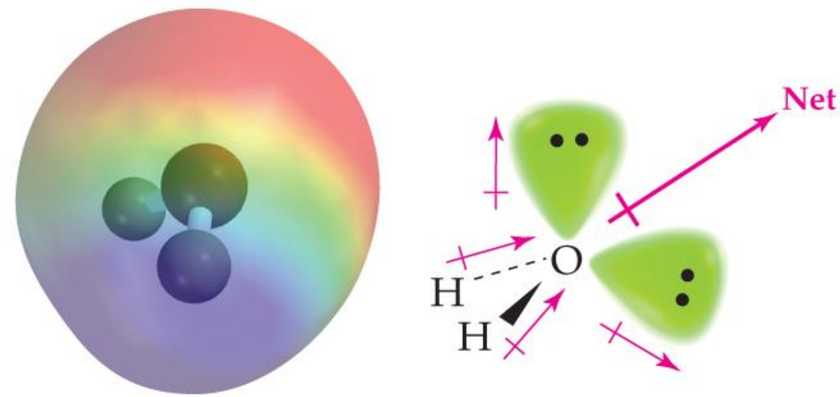
polar molecule

C—Cl bond has a **bond dipole** because of a difference in electronegativities. (Do vector sum of individual dipole moment arrows.)(If vector sum ≠ zero, then molecule is polar.)

Polar Covalent Bonds and Dipole Moments



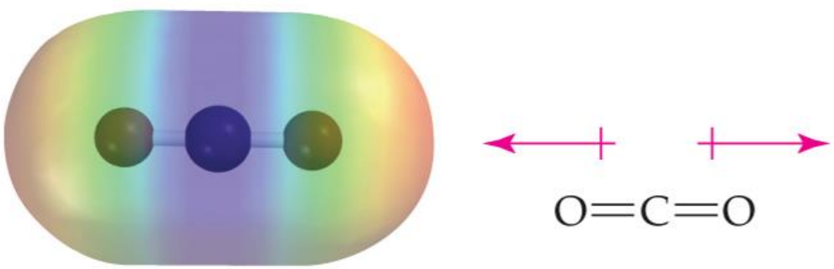
Ammonia (μ = 1.47 D)



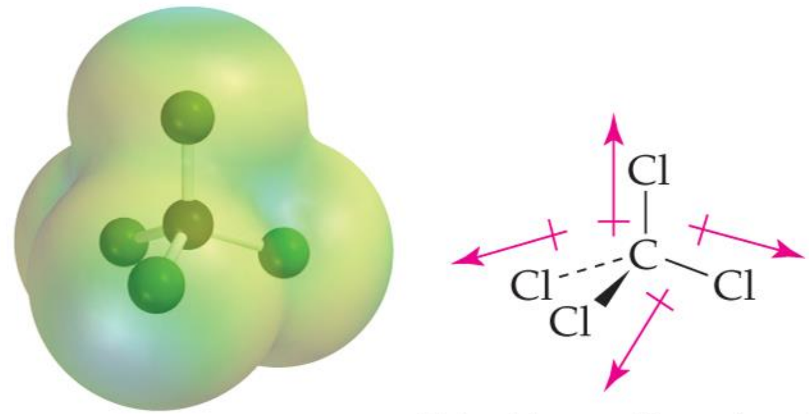
Water (μ = 1.85 D)

The individual bond polarities **do not** cancel. Therefore, the molecule has a dipole moment. In other words, the molecule is **polar**. (vector sum of individual bond dipoles ≠ zero, molecule polar)

Polar Covalent Bonds and Dipole Moments



Carbon dioxide (μ = 0)



Tetrachloromethane (μ = 0)

The individual bond polarities cancel. (vector sum of individual dipoles = zero) Therefore, the molecule does not have a dipole moment. In other words, the molecule is **nonpolar**.

Intermolecular Forces

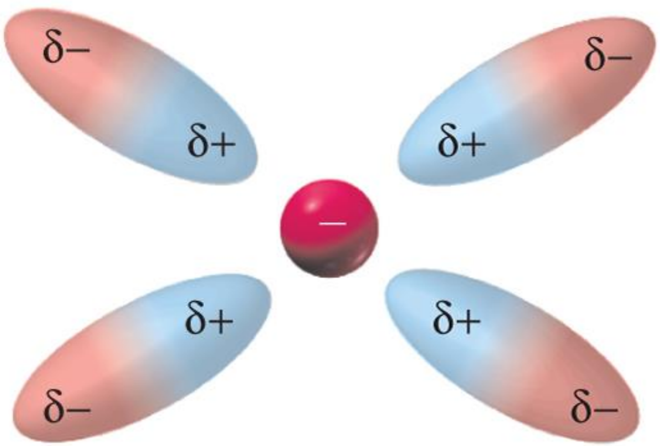
Intermolecular Forces: Attractions between "molecules" that hold them together. These forces are electrical in origin and result from the mutual attraction of unlike charges or the mutual repulsion of like charges. (like interstate highways)

Types of Intermolecular Forces (higher Intermolecular Force, higher MP/BP)

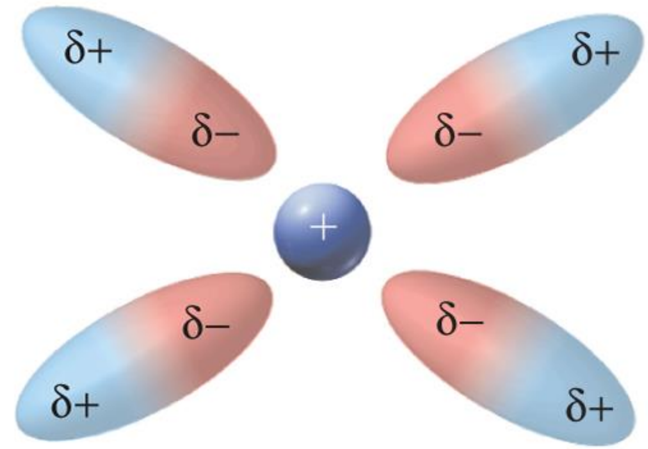
- Ion–dipole forces (variable strength)
- Van der Waals forces
  - hydrogen bonds (strongest intermolecular)
  - dipole–dipole forces
  - London dispersion forces (weakest intermolecular)

Intermolecular Forces

Ion–Dipole Forces: The result of electrical interactions between an ion and the partial charges on a polar molecule (usually found in solutions of ions in polar molecules)



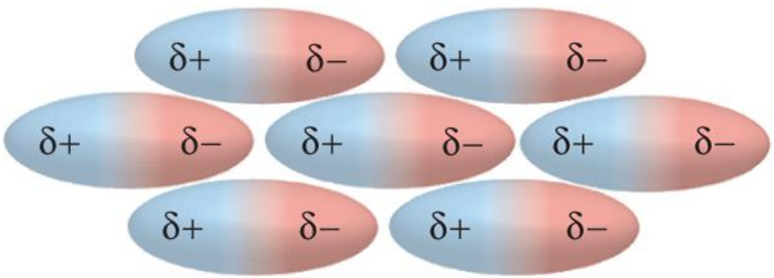
Polar molecules orient toward ions so that the **positive end** of the dipole is near an **anion** and …



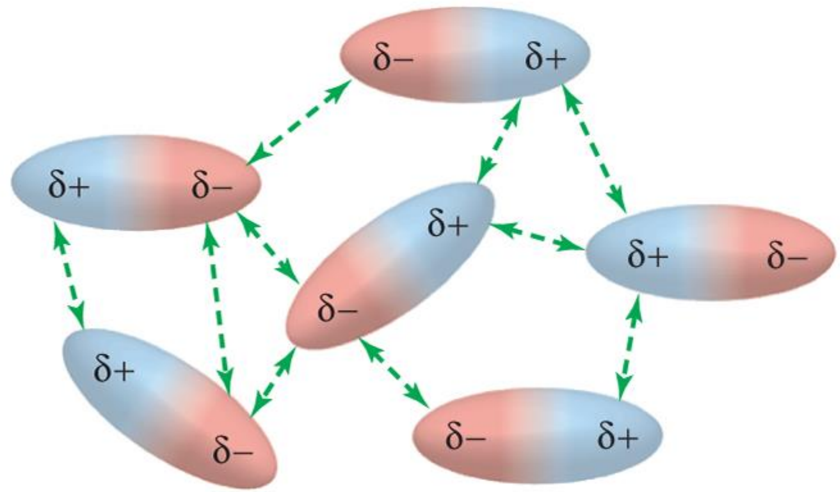
… the **negative end** of the dipole is near a **cation**.

Intermolecular Forces

Dipole–Dipole Forces: The result of electrical interactions among permanent dipoles on neighboring molecules



Polar molecules **attract** one another when they orient with unlike charges close together, but …



… they **repel** one another when they orient with like charges together.

End 11/20 Wed F section

Intermolecular Forces

Dipole–Dipole Forces

TABLE 8.4 Comparison of Molecular Weights, Dipole Moments, and Boiling Points

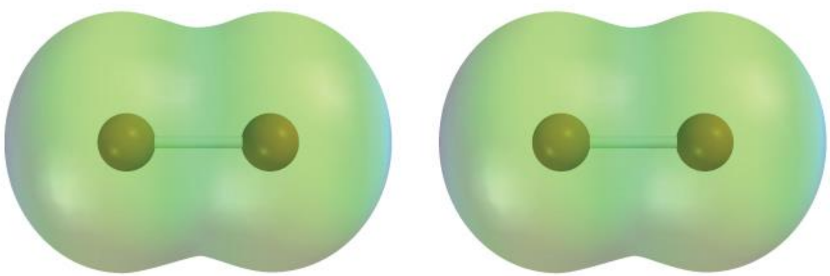
Substance		Mol. Wt.	Dipole Moment (D)	bp (K)
$CH_3CH_2CH_3$	London	44.10	0.08	231
CH_3OCH_3	dipole-dipole	46.07	1.30	248
CH_3CN	dipole-dipole	41.05	3.93	355

As the *dipole moment increases*, the *intermolecular forces increase*.

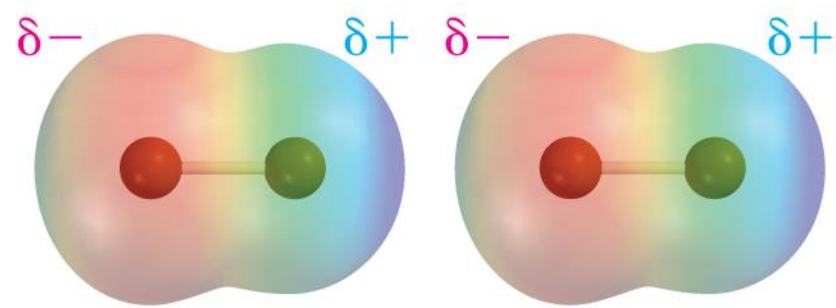
As the *intermolecular forces increase*, the *boiling point increases*.

Intermolecular Forces

London Dispersion Forces: The result of the motion of electrons that gives the molecule a short-lived dipole moment. This induces temporary dipoles in neighboring molecules. (other texts call this Van der Waals forces)



Averaged over time, the electron distribution in a Br_2 molecule is **symmetrical**.



At any given instant, the electron distribution in a molecule may be **unsymmetrical,** resulting in a temporary dipole and inducing a complementary attractive dipole in neighboring molecules.

Intermolecular Forces

London Dispersion Forces

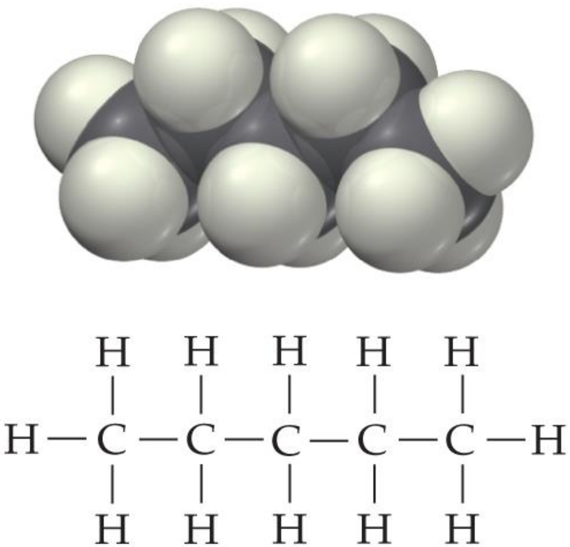
TABLE 8.5 Melting Points and Boiling Points of the Halogens

Halogen	mp (K)	bp (K)
F_2	53.5	85.0
Cl_2	171.6	239.1
Br_2	265.9	331.9
I_2	386.8	457.5

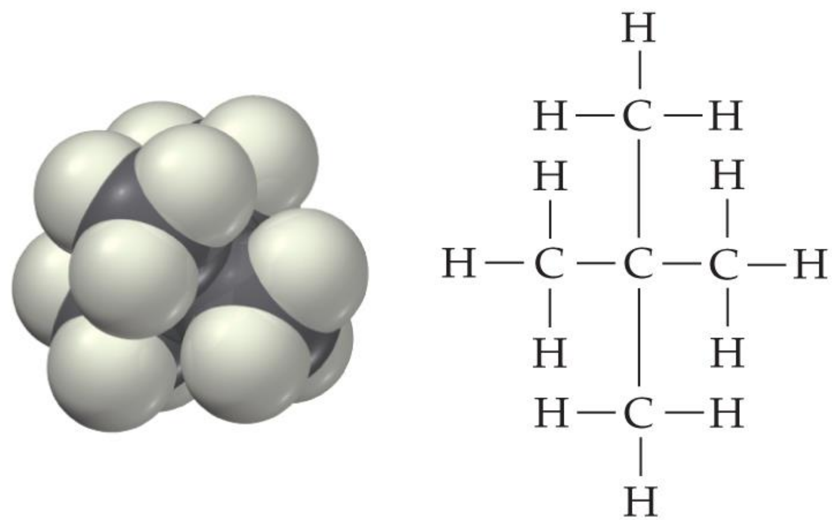
As the *dispersion forces* increase, the *intermolecular forces* increase. As the *intermolecular forces* increase, the *boiling point* increases. (larger molecules have higher London force, higher MP/BP)

Intermolecular Forces

London Dispersion Forces
(higher with higher surface area of contact)



Pentane (bp = 309.2 K)



2,2-Dimethylpropane (bp = 282.6 K)

Longer, **less compact molecules** like pentane feel stronger dispersion forces and consequently have higher boiling points.

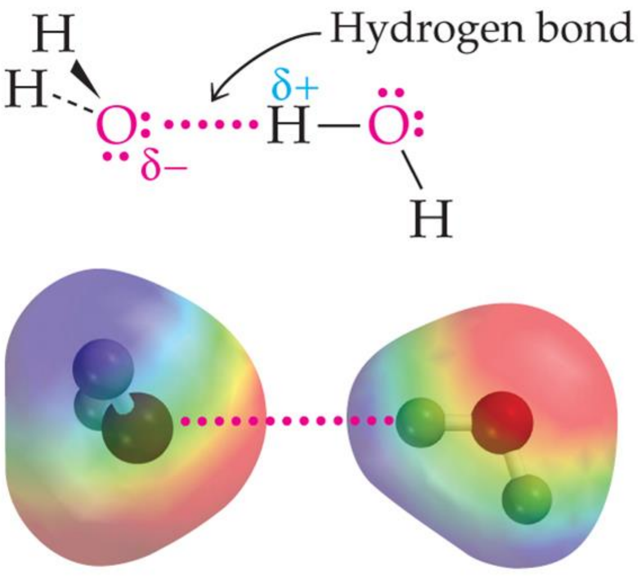
More compact molecules like 2,2-dimethylpropane feel weaker dispersion forces and have lower boiling points.

higher London, higher MP/BP

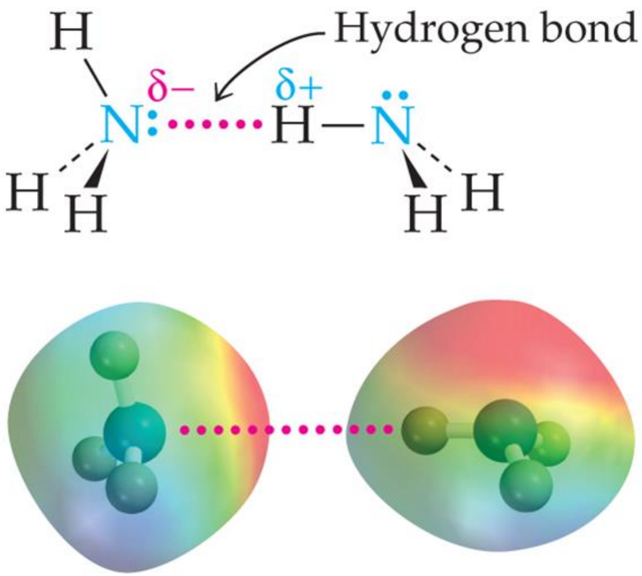
lower London, lower MP/BP

Intermolecular Forces

Hydrogen Bond: hydrogen atom directly bonded to a very electronegative atom (F, O, N) (almost FUN) and an unshared electron pair on another electronegative atom



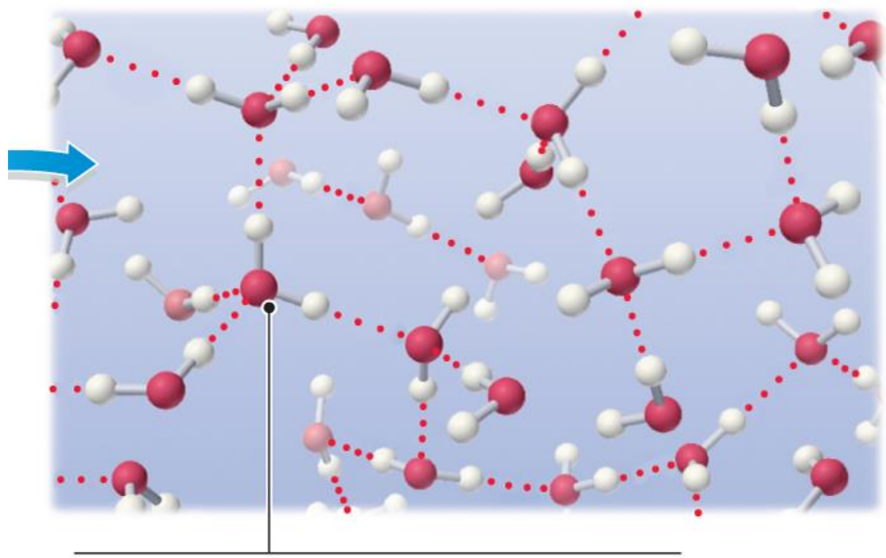
Water



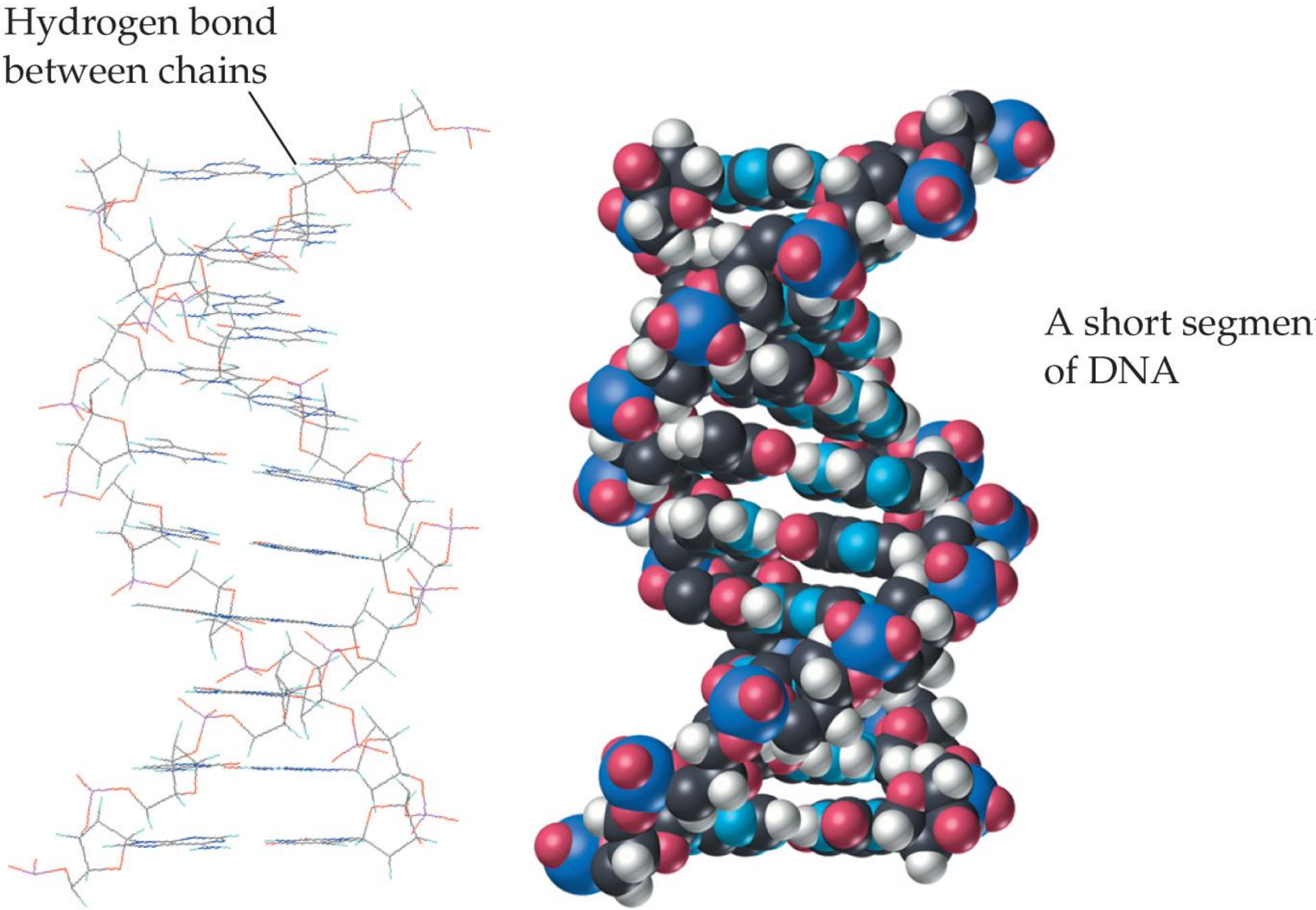
Ammonia

Hydrogen Bond

Liquid water contains a vast three-dimensional network of hydrogen bonds resulting from the attraction between positively polarized hydrogens and electron pairs on negatively polarized **oxygens**.



An **oxygen** can form two hydrogen bonds, represented by dotted lines.


Hydrogen bond between chains
A short segment of DNA

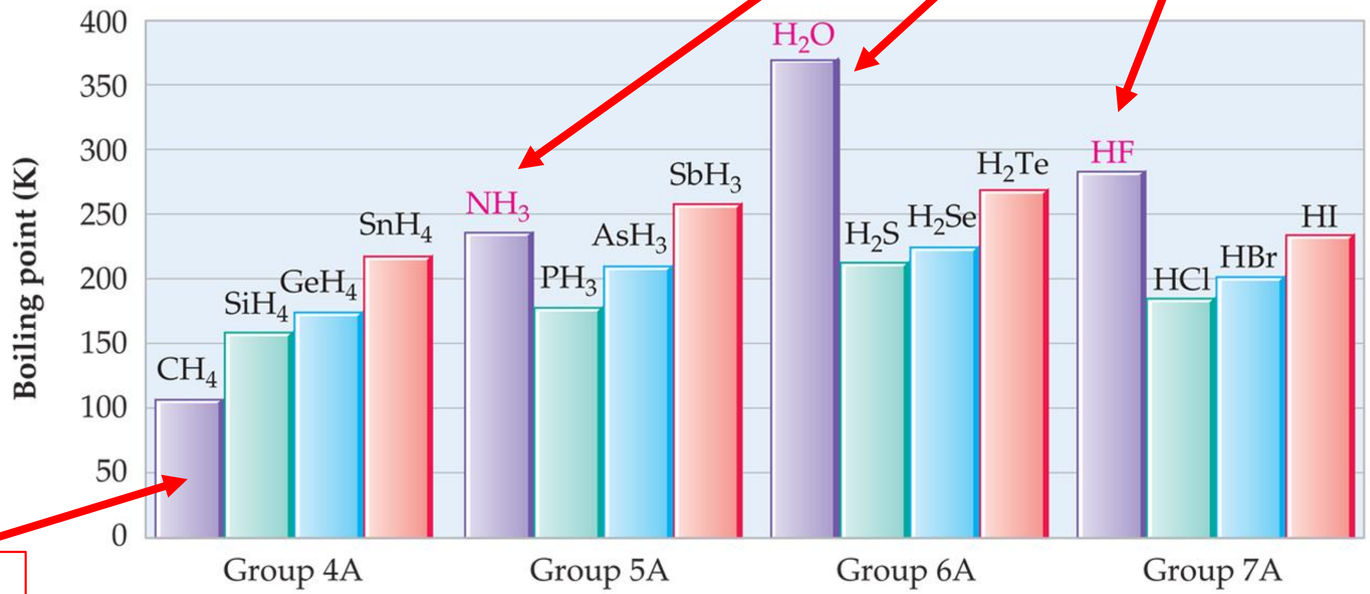
Intermolecular Forces

11/20 W G section

H bond

Hydrogen Bond

TABLE 8.6 **Boiling Points of the Covalent Binary Hydrides of Groups 4A, 5A, 6A, and 7A**



No H bond

The boiling points generally increase with increasing molecular weight down a group of the periodic table, but the hydrides of nitrogen **(NH_3)**, oxygen **(H_2O)**, and fluorine **(HF)** have abnormally high boiling points because these molecules form hydrogen bonds.

Intermolecular Forces

TABLE 8.7 A Comparison of Intermolecular Forces

Force	Strength	Characteristics
Ion–dipole	Highly variable (10–70 kJ/mol)	Occurs between ions and polar molecules
Dipole–dipole	Weak (3–4 kJ/mol)	Occurs between polar molecules
London dispersion	Weak (1–10 kJ/mol)	Occurs between all molecules; strength depends on size, polarizability
Hydrogen bond	Moderate (10–40 kJ/mol)	Occurs between molecules with O—H, N—H, and F—H bonds

ion-ion > ion-dipole > H bonding > dipole- dipole > London dispersion

Largest Intermolecular Force Smallest Intermolecular Force

Everything has London. If also has one of the other intermolecular forces (ion-dipole, dipole-dipole or H bonding) than list that as the predominant Intermolecular Force.

HW 8-4: Intermolecular Forces

Note: I now do NOT post the HW or HW answers with the posted powerpoint. You can come to class and pick up the HW powerpoint handout for in this case HW 8-4. You will have to get the answers to HW from either a fellow student who was in class OR get the answer from me by asking questions. I usually give the answer at the next class period as well.

11/21/19 Thursday end D section

End Here: Quiz 4 & Test 4 (both) (Quiz probably all Short Answer) (test 60% multiple choice, 40% short answers) Covers: All of Chapters 6,7, & 8 (up to & including HW 8.4) (remember that my section did not include any of chapter 6 on the test 3 because one section of my 3 lecture section was about 4 powerpoint slides from finishing chapter 6)

Final Exam will probably include parts of Chapter 10 All professors teaching General Chemistry I are skipping Chapter 9. All my 3 sections will probably finish Chapter 8 on Monday & maybe start Chapter 10. (I will also answer questions on any material for Quiz 4 & Test 4 on Monday)

Molecular Orbital Theory: The Hydrogen Molecule

Atomic Orbital (AO): A wave function whose square gives the probability of finding an electron within a given region of space *in an atom* *(where electrons are located in an atom)*

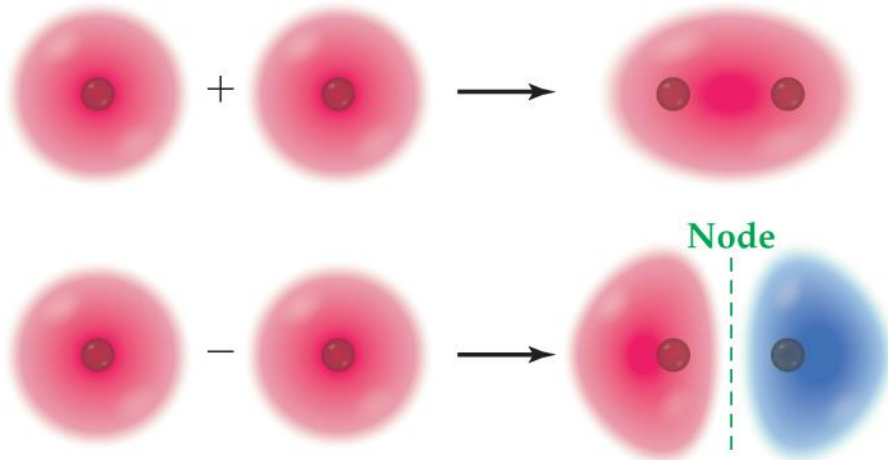
Molecular Orbital (MO): A wave function whose square gives the probability of finding an electron within a given region of space *in a molecule* *(where electrons are located in a molecule)*

Molecular Orbital Theory: The Hydrogen Molecule (combine AO to make MO)

σ bonding orbital

The additive combination of atomic 1*s* orbitals forms a lower-energy, **bonding molecular orbital**, σ.

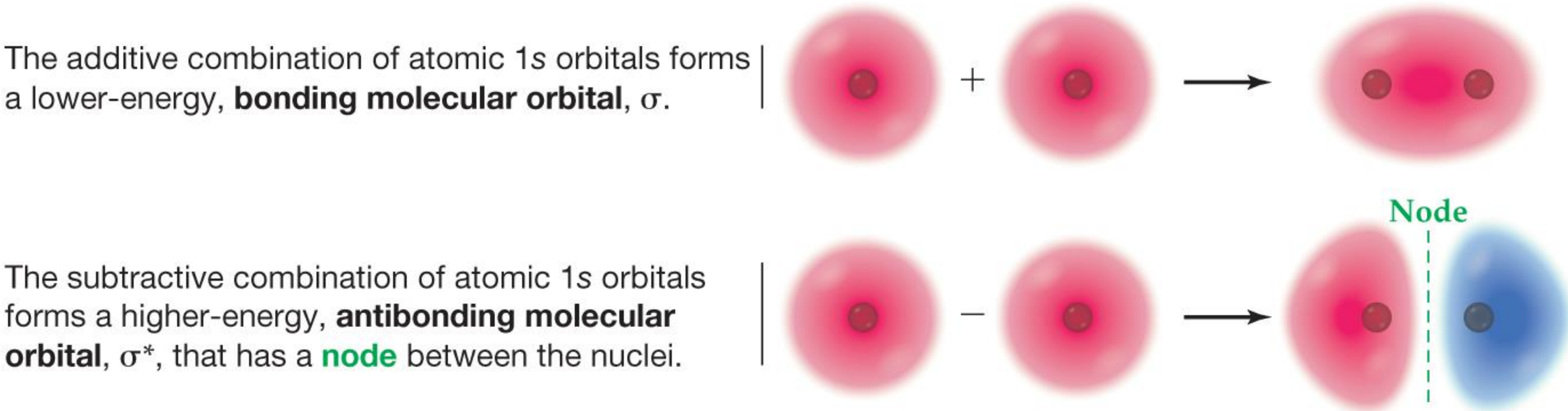
The subtractive combination of atomic 1*s* orbitals forms a higher-energy, **antibonding molecular orbital**, σ*, that has a **node** between the nuclei.



σ* antibonding orbital
higher energy

Molecular Orbital Theory: The Hydrogen Molecule

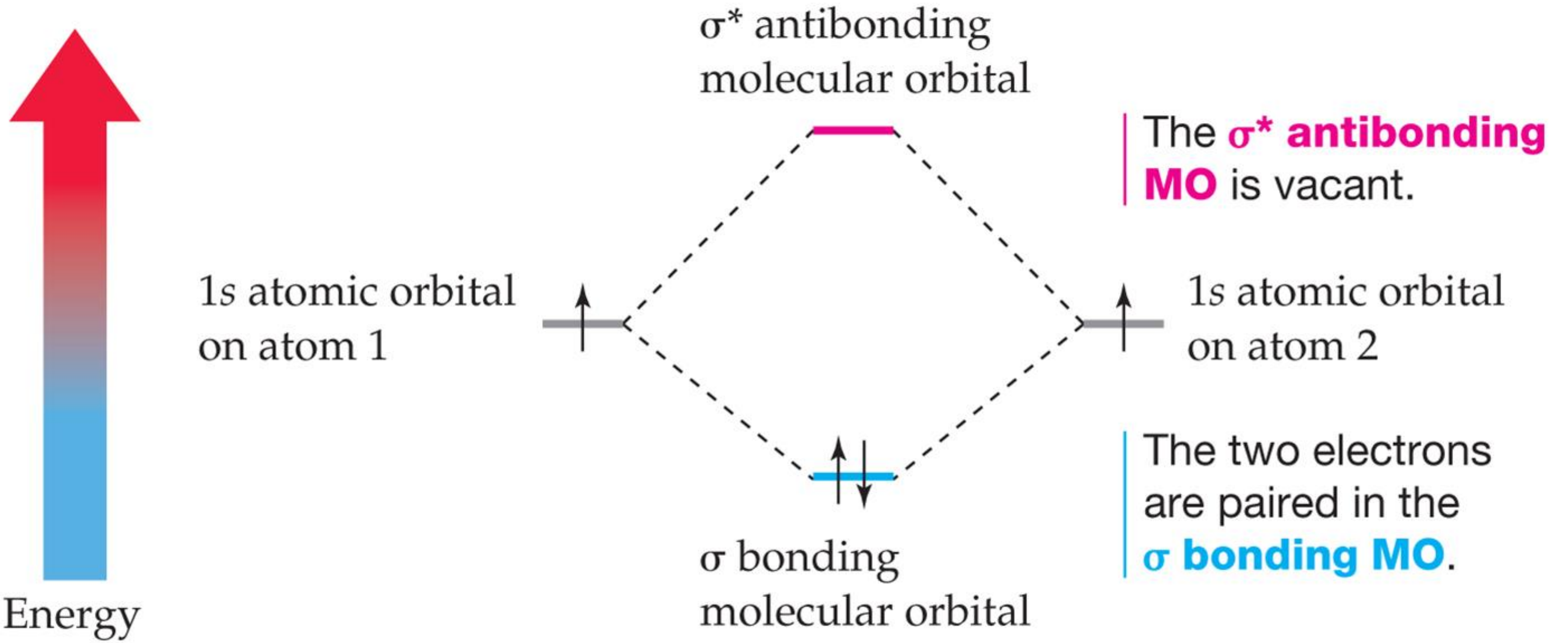
σ bonding orbital



σ* antibonding orbital

$$\text{Bond order} = \frac{(\#\text{ bonding } e^- - \#\text{ antibonding } e^-)}{2}$$

Molecular Orbital Theory: The Hydrogen Molecule (MO lower in energy than AO)



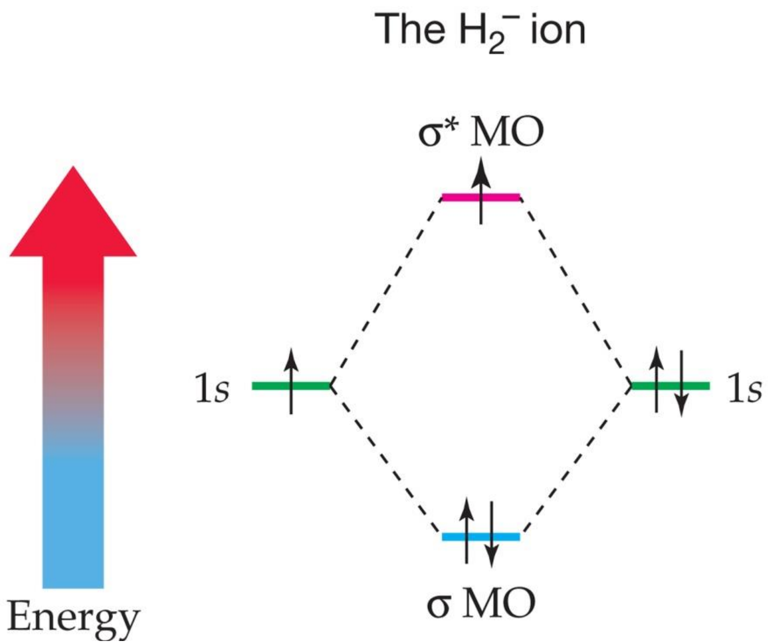
$$\text{Bond order} = \frac{2 - 0}{2} = 1$$

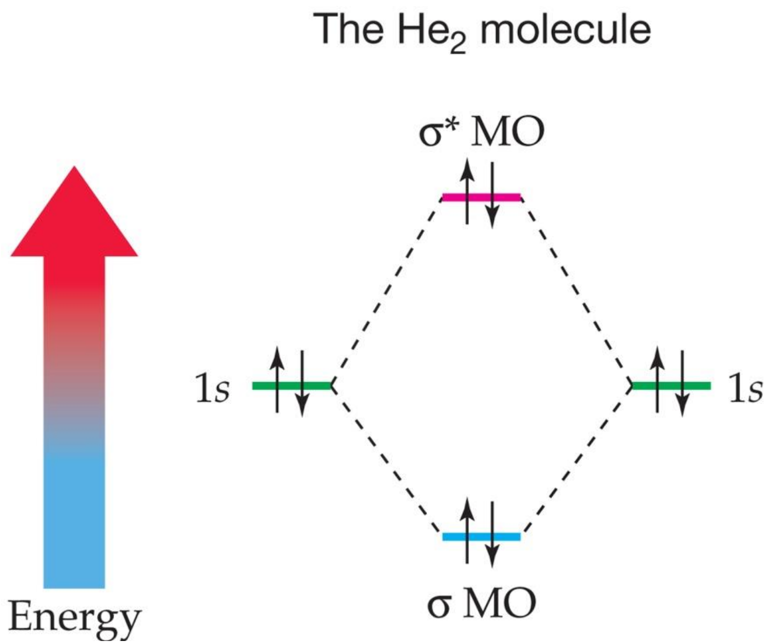
2 e is one bond

Molecular Orbital Theory: The Hydrogen Molecule

End 11/22/19
Friday F section

not stable





Bond order: $\dfrac{2-1}{2} = \dfrac{1}{2}$ $\qquad \dfrac{2-2}{2} = 0$

HW 8-5: Molecular Orbital Theory.

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G section 11/22 F